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Total System Performance Assessment-License Application Methods and Approach

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Civilian Radioactive Waste Management System
Management & Operating Contractor

Total System Performance Assessment-License Application Methods and Approach

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1. PURPOSE

Total System Performance Assessment–License Application (TSPA-LA) Methods and Approach provides the top-level method and approach for conducting the TSPA-LA model development and analyses. The method and approach is responsive to the criteria set forth in Total System Performance Assessment Integration (TSPAI) Key Technical Issue (KTI) agreements, the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]), and 10 CFR Part 63. This introductory section provides an overview of the TSPA-LA, the projected TSPA-LA documentation structure, and the goals of the document. It also provides a brief discussion of the regulatory framework, the approach to risk management of the development and analysis of the model, and the overall organization of the document. The section closes with some important conventions that are utilized in this document.

1.1 OVERVIEW OF TSPA-LA

The general total system performance assessment process has developed over time through its application on numerous projects by various international organizations involved in radioactive waste management and in consultation with the U.S. Nuclear Regulatory Commission. The TSPA must be based on a thorough understanding of the relevant processes that may affect performance, site-specific information, and relevant laboratory data concerning the engineered materials. The TSPA approach allows an analysis of the system that appropriately incorporates and quantifies the uncertainty in such a long-term projection of repository performance. The TSPA-LA aims to provide a defensible analysis of system behavior incorporating models and parameters that are based on scientific observations in order that the ability of the repository system to comply with applicable radiation protection standards can be assessed.

The TSPA process can be visualized as a series of levels going up a pyramid. The base of the pyramid is built using the data and information collected by scientists and engineers involved in site characterization and engineering design. This information is used to develop appropriate models which describe the features, events, and processes that may be present in the proposed repository system. The base is large because it represents the composite of the information gathered by the repository program over a period of more than 20 years. This information provides the basis for the development and testing of conceptual models. A conceptual model is a set of hypotheses (including assumptions, simplifications, and idealizations) used to describe the essential aspects of a system or subsystem for a given purpose. An example is a description of the movement of water molecules as they move in rock pores or fracture openings. There may be several alternative conceptual models that provide a reasonable description of a particular system or subsystem.

The specific aspects for describing a process on a larger scale are then extracted and incorporated into computer models to deal with each of the relevant features, events, and processes. An example is a model for all water flow above the water table, which would incorporate flow interactions between the rock matrix and the rock fractures as well as many other specifics needed to describe how water flows throughout the rock mass. This abstraction or progressive simplification to a more compact and usable form is depicted by the slightly smaller width of the pyramid. The models that eventually analyze the evolution through time of all the various components of the system are generally the most compact or abstracted models of all. These abstracted models start with the results of the detailed process level modeling and create a representation that captures all the salient features of the process model, and the associated uncertainties.

To capture the full detail of the uncertainty and variability in the behavior of the repository system, the total system performance assessment must be probabilistic, using multiple calculations (as opposed to deterministic or a single calculation using a single value for each parameter in the system). The models are run many times using many combinations of parameters. Each of the combinations of parameters has some definite possibility of representing the actual performance of the proposed repository. These probabilistic analyses are intended to reflect the range of behaviors or values for parameters that could be appropriate, knowing that perfect or complete knowledge of the system will never be available and that the system is inherently variable.

The aspects of the total system performance analyses to be contained in the TSPA-LA model and documentation are defined in several sources including the features, events, and processes (FEPs) analyses, KTI agreements, the current draft of the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]), and 10 CFR Part 63. In addition, the TSPA-LA model and documentation will build on and address issues raised in the previous iterations of TSPAs for Yucca Mountain and by additional reviews, both internal and external (e.g., U.S. Nuclear Waste Technical Review Board, and Performance Assessment International Review Team (*An International Peer Review of the Yucca Mountain Project TSPA-SR, Total System Performance Assessment for the Site Recommendation* (OECD and IAEA 2002 [158098])).

The TSPA-LA documentation structure consists of the TSPA-LA Model Document and the TSPA-LA Analysis Document (see Figure 1.1-1). These documents support the portions of the License Application documentation that describe the postclosure performance of the system. There are a large number of supporting documents as well, shown on the figure as Analysis and Model Reports (AMR). The figure also depicts four major blocks of time: (1) producing the inputs and supporting AMRs (through May 2003), (2) developing the TSPA-LA Model Document including theory, testing, and validation, (3) developing the TSPA-LA Analysis Document including the compliance analyses, and (4) supporting the License Application document (primarily Chapter 2).

The following describes the general content of these TSPA-LA documents.

- **TSPA-LA Model Document**-This documentation will follow project procedure AP-SIII.10Q*, Models,* and provide information about the TSPA-LA model. The documentation will include both a summary paper copy of top-level information about the model, as well as annotations in the model file itself. The latter will allow the reviewer to view various components of the model, and then link to the appropriate supporting information for ease of traceability. This approach will also reduce the potential for transcription errors from the TSPA-LA model file in the TSPA software to the summary paper copy. The paper documentation will discuss the conceptual model, software architecture, inputs, assumptions, and model testing. A key part of the documentation will be the discussion on the validation or confidence in the model.

- **TSPA-LA Analysis Document**-This document will follow AP-SIII.9Q*, Scientific Analyses,* and will provide the analyses of the postclosure performance of the repository system to assess compliance with appropriate regulations. As such, the detailed analyses of the simulations (both individual and multiple realization results) will be presented. The document will discuss the results from the scenario classes, and provide uncertainty importance analyses of the results. Multiple barrier discussion will also be provided in this document.

In addition to the two TSPA-LA specific documents just described, the hierarchy of AMRs provide the underlying basis for the TSPA-LA model. Further, the FEPs database and associated documentation are an integral part in the overall documentation. These will be described in numerous FEP documents (one for each major component of the model), and in a database summary document. *The Enhanced Plan for Features, Events, and Processes (FEPs) at Yucca Mountain,* (hereafter referred to as *Enhanced FEPs Plan*) developed in 2002 (BSC 2002 [158966]) describes the overall approach to this documentation. The major aspects of the plan are summarized later in this document (Section 3.2).

Information from the TSPA-LA documentation suite will be utilized to provide the appropriate information for the LA documentation. The LA documentation is expected to synthesize and provide the TSPA analyses at a general level, less detailed than that provided in the TSPA-LA documentation.

1.2 GOALS OF THE TSPA-LA METHODS AND APPROACH DOCUMENT

Specific goals of the TSPA-LA Methods and Approach document are:

- To describe the upper-level approach and processes for development and testing of the TSPA-LA model, and its documentation, in a controlled environment. The basis for the type of analyses to be developed will be determined from the U.S. Nuclear Regulatory Commission (NRC) regulation (10 CFR Part 63), the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]), and KTI agreements.
- To describe the systematic approach to collecting and utilizing information (e.g., data, abstractions) from the supporting organizations. In particular, the consistent treatment and documentation of FEPs, model abstractions, alternative conceptual models (ACMs), and parameters and their uncertainty are described.
- To provide a brief approach to ensure the TSPA-LA model and documentation are traceable and transparent to potential users of the information. The approach builds on the data tracking, model checking, and graphical representation of information that have been used in previous TSPAs.
- To provide the approach for the analysis of barriers with the TSPA-LA model.
- To provide limited documentation of the changes in the approach from the TSPA-SR to the TSPA-LA, such as model components, scenario classes, and sensitivity analysis techniques.

- To provide summary-level guidance to the science and design elements within the project regarding inputs that will be required for the TSPA-LA.
- To incorporate comments from external reviewers in the modeling approach.

Three important caveats apply to these goals:

1. The *TSPA-LA Methods and Approach* document should not be viewed as a final design document for the TSPA-LA. Rather, it provides documentation of the current approach, and an early opportunity for comment. The final design of the TSPA-LA may differ from what is described in this document.
2. The information contained in this document regarding the configuration of the model and the plans for further development must be understood to be preliminary and interim. The technical integration work necessary to finalize the inputs and the character of the abstractions to be utilized in the TSPA-LA is ongoing.
3. The controlling Administrative Procedures supercede any guidance provided in this document. If conflicts between this document and applicable procedures are identified, this will be immediately raised to the appropriate responsible manager.

1.3 REGULATORY FRAMEWORK

A licensing requirement for the disposal of high-level radioactive waste at the proposed Yucca Mountain geologic repository is the evaluation of postclosure performance. The NRC, in their regulation 10 CFR Part 63, requires that a performance assessment analysis be performed for this evaluation. A performance assessment is defined as (10 CFR 63.2) "an analysis that:

(1) Identifies the features, events, processes (except human intrusion), and sequences of events and processes (except human intrusion) that might affect the Yucca Mountain disposal system and their probabilities of occurring during 10,000 years after disposal;

(2) Examines the effects of those features, events, processes, and sequences of events and processes upon the performance of the Yucca Mountain disposal system; and

(3) Estimates the dose incurred by the reasonably maximally exposed individual [RMEI], including the associated uncertainties, as a result of releases caused by all significant features, events, processes, and sequences of events and processes, weighted by their probability of occurrence."

The NRC regulation (10 CFR Part 63) forms the basis for the regulatory framework guiding the development of the TSPA-LA model, and subsequent TSPA analyses for the LA. The regulatory time period of analysis for the compliance evaluation is 10,000 years. However, the TSPA analyses are intended to extend beyond 10,000 years to 20,000 years. This is intended to provide a basis for evaluating whether uncertainties in results after 10,000 years affect conclusions regarding compliance during the regulatory performance period. Likewise, the FEPs for these analyses will not go beyond 10,000 years. The TSPA for the Final Environmental Impact

Statement (FEIS) (hereafter referred to as TSPA-FEIS model) evaluated doses over longer time periods (up to 1 million years).

1.4 RISK MANAGEMENT

The development and documentation of the TSPA-LA requires coordination and integration with a large number of project resources. This complexity adds risk to the process of developing and documenting the model; risk in terms of technical risk as well as schedule risk. Inputs need to be delivered in appropriate form and on time to support the TSPA-LA model development. Testing and validation of the developing model needs to be accomplished in the appropriate time frame to support analyses and documentation in the LA. Late-changing external requirements also need to be managed appropriately to avoid compromising the planned technical and schedule goals.

To support the reduction of input risks (e.g., late receipt of abstractions, delays in qualification of supporting data, etc.), the schedule for receipt of inputs is being closely managed with weekly critical path meetings. As delays are encountered, the situation is rapidly assessed and an alternative approach to the activity is put in place. This may mean that the type and volume of new or updated information to be incorporated into the TSPA-LA will be changed. This will be assessed on a case by case, risk-informed basis, with the potential modification of the uncertainty in a particular component being an outcome (e.g., a distribution may need to be modified to account for additional uncertainty). Consistency of data feeds (parameters, abstractions, FEPs, uncertainty) is being built into the development process (see Section 3). Integration of these data feeds with the TSPA requirements will be accomplished through ongoing communication with the appropriate organizations.

Software qualification is another potential source of risk to successful completion of a TSPA-LA model. The procedure for software qualification, AP-SI.1Q, *Software Management*, is currently undergoing revision and should provide a streamlined approach to qualification of updates to software. The TSPA-LA model will be based primarily on existing software utilized during the site recommendation process, so there will be a limited number of cases with completely new software, as opposed to updated software.

The potential for discovery of errors in TSPA-LA at a late date exists. The primary approach to reduce the risk from such occurrences is to build in quality from the outset. Enhancements to the processes for development, checking, and testing of the model and its documentation have been developed based on lessons learned in the development of the TSPA-SR (See Section 6 for details). The thoroughness in checking and testing of any model changes are likely to enhance the potential for early discovery of any potential errors in the TSPA-LA.

Additional risks (e.g., computer crashes, late changes in types of analyses required, etc.) will be managed in a preemptive fashion when possible. Recovery plans are in place for loss of data (Dunlap 2002 [159697]). Modularization of the model will help analysts remain flexible to analysis changes that are required at a later date. However, unforeseen complications in the development of the model or analyses will need to be managed as they arise, and may entail scope changes (i.e., reduction to recoup schedule), schedule changes (e.g., increasing schedule time for particular activities, or making previously sequential activities occur in parallel), or modification of staffing levels.

The TSPA-SR model and documentation underwent significant evaluation and review. There were a number of issues raised with that documentation set (Doering 2001 [156966]; BSC 2001 [156961]; Hosmer and King 2001 [157923]; and BSC 2001 [158980]). The issues included documentation errors (e.g., typos, referencing errors, clarity) and modeling discrepancies. Process steps have been taken to mitigate the issues in this next iteration of the TSPA (See Section 6 for model development processes).

1.5 ORGANIZATION OF THE DOCUMENT

This Methods and Approach Document contains information intended to provide the strategy and a top-level description of how the TSPA-LA model and analyses will be developed and documented. The sections of the document are organized as follows.

- **Section 2. Quality Assurance -** This section discusses the general configuration management of data, software, and models to be utilized in developing the TSPA-LA.
- **Section 3. Processes for TSPA-LA -** The approach to consistent development of parameters, abstractions, alternative conceptual models, and uncertainty from supporting organizations is briefly described in this section. The process is described in more detail in the *Guidelines for Developing and Documenting Alternative Conceptual Models, Model Abstractions, and Parameter Uncertainty in the Total System Performance Assessment for the License Application* (BSC 2002 [158794]).
- **Section 4. Scenario Classes for LA -** The scenario classes, and the corresponding modeling cases, for TSPA-LA are described in this section. The scenario classes are (1) nominal scenario class, and (2) disruptive event scenario classes (igneous and seismic). The modeling cases in the igneous scenario class are the volcanic eruption modeling case and the igneous intrusion groundwater transport modeling case. The primary modeling case for the seismic scenario class considers extreme vibratory ground motion. Fault displacement may be included in the extreme vibratory ground motion modeling case if it is screened in for TSPA-LA , or it may be treated as a separate modeling case.
- **Section 5. TSPA-LA Model Components -** The current approach and architecture for the TSPA-LA model components are described in this section. The use of scenario classes in TSPA-LA is also described.
- **Section 6. Control of the TSPA-LA Model -** The TSPA-LA model development, testing, and analysis will be controlled using a desktop process currently undergoing review. The process will implement controls to reduce the potential for significant errors in the development of the model. This section describes this process.
- **Section 7. TSPA-LA Model Validation -** The approach to validation of the TSPA-LA model is presented in this section. Successful validation, or confidence in the TSPA-LA model, will require a substantial effort, both from the abstraction modelers and the TSPA modelers. The section details the approach to enhance confidence in the model and the approach to evaluation of the stability and reliability of the TSPA results.

- **Section 8. TSPA-LA Analyses -** The types of analyses to be conducted for the TSPA-LA are described in this section. Example figures are also provided. Detailed lists of simulations are provided in Appendix E. The section also specifically describes the multiple barrier analyses to be conducted.
- **Section 9. Summary -** This section provides a brief summary highlighting aspects important to the success of the document, and to subsequent TSPA-LA model development and documentation, and to the subsequent TSPA-LA analysis and documentation.
- **Section 10. References -** This section consists of references for cited documents, codes, standards, regulations, and procedures.

The following appendices are included:

- **Appendix A. Acronyms -** This appendix includes a list of key acronyms used in this document.
- **Appendix B. NRC/DOE KTI Agreements Addressed in this Document -** This appendix presents the KTI agreements that are addressed in this document, including TSPAI 1.01, TSPAI 1.02, TSPAI 4.01, TSPAI 4.03, and TSPAI 4.05 (Meserve 2001 [156977]) and indicates where in the document the KTI is addressed.
- **Appendix C. TSPA-LA Model Document Outline -** The TSPA-LA model will be described in a TSPA-LA Model Document, including inputs, outputs, and validation of the model. The table of contents for the model document is presented in this appendix. The content may change as the development of the TSPA-LA proceeds.
- **Appendix D. TSPA-LA Analysis Document Outline -** The table of contents for the TSPA-LA Analysis Document is included in this appendix. The content may change as the development of the TSPA-LA proceeds.
- **Appendix E. TSPA-LA Simulation List -** This appendix outlines the types of simulations to be conducted for the TSPA-LA, and gives as much detail about those simulations as is known at the time of completion of this document.
- **Appendix F. Example TSPA-LA Input Parameter Table -** This appendix provides a tabular listing of example input for the model.
- **Appendix G. TSPA-LA Document Hierarchy -** The appendix provides tabular and graphical depiction of the primary supporting documents for the TSPA-LA.

1.6 OTHER IMPORTANT CONVENTIONS UTILIZED IN THE DOCUMENT

An important consideration for this document is that it presents the methods and approach for, rather than results of, the TSPA-LA. It provides planning guidance to assist TSPA-LA personnel and supporting organizations in developing, analyzing, and documenting the TSPA-LA model. As noted in several places in the document, the plans for TSPA-LA may change and require modification to the approach presented herein. Also, the guidance is currently being evaluated in terms of what part of the guidance may be proceduralized, if any. The detailed approach indicated herein is intended to implement the primary Administrative Procedures used to develop and analyze the TSPA. The forms and checklists provided to assist in this process (some examples are provided later in this document) are provided merely as example forms for the type of information that needs to be recorded as the model development and analyses progress.

This report contains several conventions to facilitate transparency of the documentation. The Document Input Reference System (DIRS) numbers are associated with references cited in the text of this document. An example for the Technical Work Plan is BSC 2002 [159071]. Exceptions for the use of DIRS numbers in the text are for regulations (e.g., 10 CFR 63.2), administrative procedures (AP) (e.g., AP-SIII.10Q), and software (e.g., STN: 1000-4.06-00). Unless otherwise specified, references to software are not referring to a specific version, but direct the reader to an appropriate user's manual or the current software configuration management listing. Only the first occurrence of software references include the DIRS. The DIRS numbers are included in Section 10 for all references. In addition, the reference list is sorted by the DIRS numbers. Appendix G contains information about documents currently planned to be developed for LA, in support of the TSPA-LA. The documents listed in Appendix G are not yet developed, and thus do not have DIRS numbers and are not included on the reference list, unless an SR version of the document exists and is referenced elsewhere in this document.

The previous TSPA iteration for the Site Recommendation included a suite of models and analyses beginning with the TSPA-SR, with additional development for the Supplemental Science and Performance Analyses (SSPA) and subsequent changes to evaluate the final Environmental Protection Agency (EPA) standard. The incorporation of the final EPA standard, 40 CFR Part 197, and the analysis of the effect of changes introduced as the rule was finalized are presented in the *Total System Performance Assessment- Analyses for Disposal of Commercial and DOE Waste Inventories at Yucca Mountain – Input to Final Environmental Impact Statement and Site Suitability Evaluation* (Williams 2001 [157307].

The Total System Performance Assessment (TSPA) analyses conducted and documented prior to promulgation of the NRC final rule 10 CFR Part 63, were based on the NRC proposed rule (64 FR 8640 [101680]). Slight differences exist between the NRC's proposed and final rules which were not within the scope of the TSPA-FEIS Report (Williams 2001 [157307]), or the Preliminary Site Suitability Evaluation (PSSE) (DOE 2001 [155734]), and the documents supporting these reports. These differences include (1) the possible treatment of "unlikely" features, events and processes (FEPs) in evaluation of both the groundwater protection standard and the human-intrusion scenario of the individual protection standard, and (2) the definition of the water demand of the RMEI. Additional sensitivity analyses to support the Site Recommendation were developed to evaluate the impact of these regulatory differences on the post-closure performance assessment results previously conducted. The results of those sensitivity analyses are documented in the *Total System Performance Assessment Sensitivity Analyses for Final Nuclear Regulatory Commission Regulations* (Williams 2001 [156743]). Those sensitivity analyses indicated that although the numerical results of the previous TSPAs changed slightly, once the requirements of the NRC final 10 CFR Part 63 were incorporated into updates to the technical bases for the TSPA, the overall conclusions of the analyses were the same.

The suite of models and analyses that formed the bases for the SR iteration of the TSPA are now being fully updated to comply with the final 10 CFR Part 63, conform to the guidance in the *Yucca Mountain Review Plan* (CNWRA 2002 [158449], and address NRC Key Technical Issue Agreement Items. The potential updates to the bases for the TSPA-LA are outlined in Section 5 of this report. The TSPA-LA will then be completed based on those updates.

The updates do not represent wholesale revision to the TSPA-SR; rather, they generally correspond to work intended to enhance confidence in the results of the TSPA-SR. The work comprises efforts to enhance confidence in the results of TSPA-SR, either through incorporation of additional data, or refinement of models, including, for example, more detailed models where bounding approaches might have been used previously. The work reflects Key Technical Issue agreements with the NRC staff, which are also designed to enhance confidence in the TSPA calculations and their bases. The updates also will be responsive to the continued evolution of the program's technical bases, and incorporate, as appropriate, further enhancements defined as the program moves toward completion of the license application documentation.

The starting point for the TSPA-LA model configuration and change control is the TSPA-FEIS model, the final model in the suite developed for the Site Recommendation; however, the model contains few changes beyond what is in the TSPA-SR and the uncertainty analysis based model for the SSPA. So, the convention to be used in this document is to call the full suite of modeling and analysis the TSPA-SR, but the model file itself that is being updated for the TSPA-LA is the TSPA-FEIS model file.

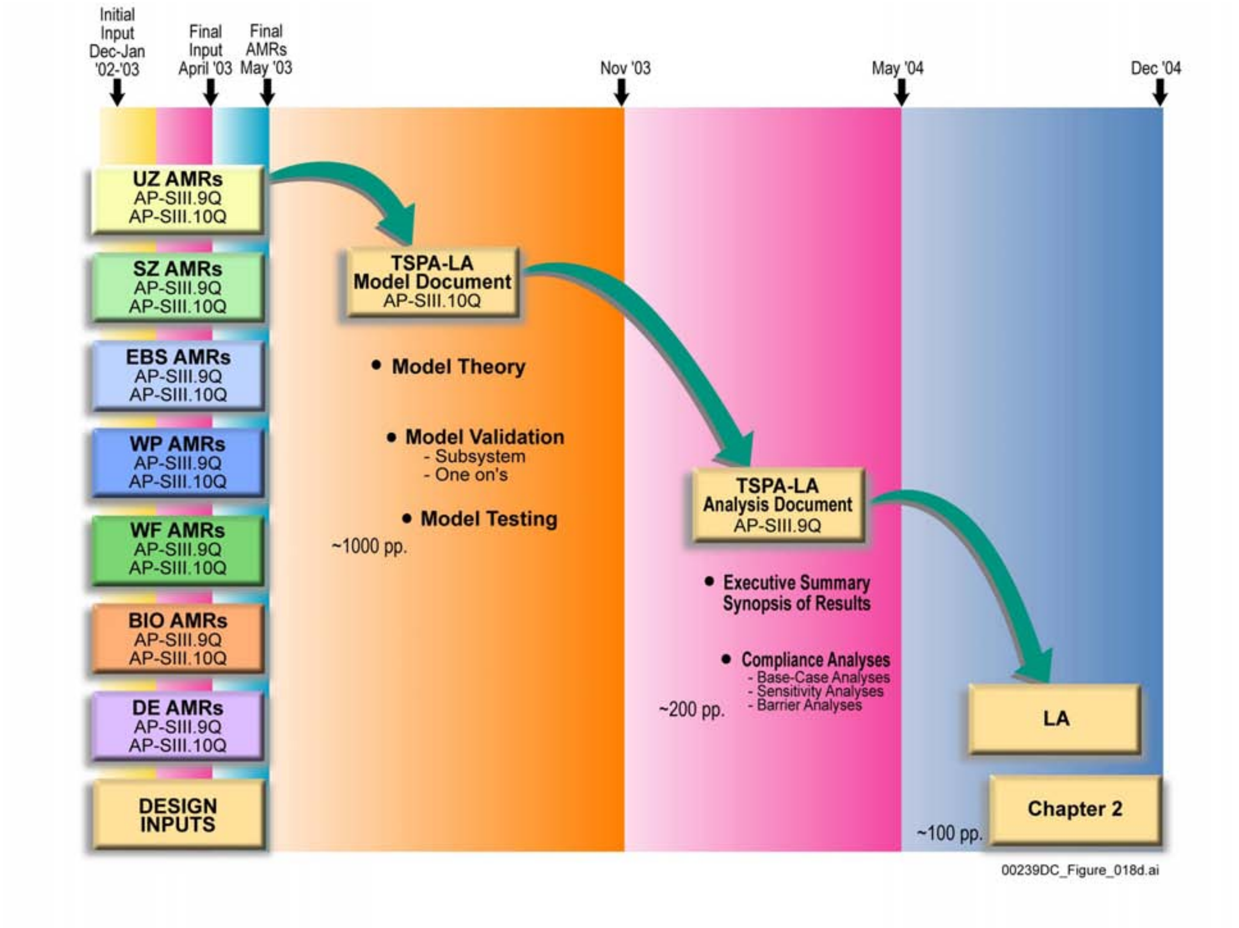


Figure 1.1-1. TSPA-LA Documentation Hierarchy

2. QUALITY ASSURANCE

Following appropriate, controlled processes and procedures is paramount to developing a traceable and defensible TSPA-LA model and analysis. Accordingly, the Quality Assurance (QA) Program applies to the development of the TSPA-LA Methods and Approach Document. The TSPA responsible manager has evaluated the technical document in accordance with AP-2.21Q, *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities.* The AP-2.21Q activity evaluation has determined that the preparation and review of this technical document is subject to the requirements in *Quality Assurance Requirements and Description* (DOE 2002 [159475]). As such, this document was developed, checked, and reviewed in accordance with AP-3.11Q, *Technical Reports*. Note that AP-2.21Q has been superceded by AP-2.27Q, *Planning for Science Activities*, and the technical work plan for this document will be updated accordingly.

The control of electronic management of data was also evaluated in accordance with AP-SV.1Q, *Control of the Electronic Management of Information* in *Technical Work Plan for: TSPA-LA Methods and Approach Document* (BSC 2002 [159071]). The evaluation determined that the current work practices and procedures are adequate for the control of electronic management of data for this activity.

In addition, an important part of the process for developing the TSPA-LA is appropriate configuration management. Configuration management is the process of identifying and defining the configuration items in a system, controlling the release and change of the items in the system, reporting the status of the items in the system, and verifying the completeness and correctness of the items in the system. The first process in the configuration management system called configuration identification is the unique identification of all the items to be managed in the system. Configuration identification consists of selecting the items to be managed and recording their functional and physical characteristics. The second process is configuration change control. Configuration change control is the mechanism for approving or disapproving all proposed changes to the system that is being managed. Configuration change control ensures that changes to any configuration items are approved and controlled so that consistency among components is maintained. The TSPA responsible manager will manage any proposed changes to the TSPA-LA model. The third process is called configuration status accounting. Information contained in the status accounting system will document the evolution of the TSPA-LA model in a transparent and traceable manner. The last process is review. The review consists of checking the configuration items to verify that they match the requirements. It is anticipated that the TSPA-LA model will undergo several technical and QA reviews prior to qualification per the applicable Administrative Procedures (AP). Configuration management for software, model, and model inputs utilized in TSPA-LA model are discussed in the following subsections.

2.1 SOFTWARE CONFIGURATION MANAGEMENT

All software codes used to support the TSPA-LA model will be qualified and placed under the controls of the software configuration management (SCM) program per AP-SI.1Q, *Software Management*. Procedurally, qualified software is software that has successfully completed the verification and validation phases but has not been baselined. Baselined software is software that has been formally reviewed, can only be changed through a formal change process, and is ready for project use. Each qualified software code in Software Configuration Management (SCM) is uniquely identified with a tracking number. The SCM database also includes information on the software name, version, and operating platform it was qualified for. All software documentation including the media will be linked to this unique software tracking number, which will allow cross-referencing of the baseline elements to the overall software qualification package.

To support the TSPA-LA model, a number of software codes will be implemented. The codes will be used for both providing supporting information, and directly implementing the TSPA-LA model. The former software codes are referred to as process models and are developed and operated external to and prior to running the TSPA model. The latter software codes are generally referred to as abstractions, and are run directly within the TSPA model. This document is focussed on the TSPA-LA model, with less emphasis on those external process models though they are mentioned for completeness.

The TSPA-FEIS model will be used as the basis for the TSPA-LA model. Currently the TSPA-FEIS model contains both qualified and unqualified software, and is the culmination of the work done for the TSPA-SR, Supplemental Science and Performance Analyses, and the FEIS. During initial TSPA-LA model development, changes to the TSPA-FEIS model and the associated software codes are expected to occur, which are discussed in Section 5.1. Some new software may be developed or older versions of codes updated.

The software codes for the TSPA-FEIS model are listed in Table 2.1-1 (see Williams 2001 [157307]). The SCCD and WAPDEG were updated from the versions used in the SSPA (BSC 2001 [154659]), Section 2.3-1). A brief description of the primary function of the software is also provided in this section. The documentation for each code is available in SCM. Unless noted, the codes described below are directly linked to GoldSim during the TSPA analyses.

Table 2.1-1. TSPA-FEIS Software Codes

Code and Version	Software Tracking Number
GoldSim V 7.17.200	STN:10344-7.17.200-00
ASHPLUME V1.4LV.dll	STN:10022-1.4LV-dll-00
CWD V1.0	STN:10363-1.0-00
FEHM V2.10NT	STN:10086-2.10-02
GVP V1.02	STN:10341-1.02-00
MKTable V1.0	STN:10505-1.00-00
Patch_Fail_Lag V1.0	STN:10532-1.0-00
SCCD V2.01	STN:10343-2.01-00
SEEPAGEDLLMK2_UU V1.0	STN:10534-1.0-00
SOILEXP V1.0	STN:10492-1.0-00
SZ_Convolute V2.1	STN:10207-2.1-00
WAPDEG V4.06	STN:10000-4.06-00

Note: The software listed in this table was utilized for the TSPA-FEIS analyses documented in Williams (2001 [157307]).

GoldSim - GoldSim is a Windows-based program that is the modeling software for simulating the TSPA-LA model. Probabilistic simulations are represented graphically in GoldSim. Models are created in GoldSim by manipulating graphical objects, where these objects represent the features, events, and processes (FEPs) controlling the system being simulated. GoldSim is flexible in its ability to incorporate a variety of data tables, other software modules, and information in defining the overall system model.

ASHPLUME - This software will be used to model volcanic ash dispersion and deposition to evaluate the consequences of extrusive volcanic events through the proposed repository. The software estimates the distribution of ash and radioactive waste released into the biosphere during hypothetical volcanic events that intersect the repository. ASHPLUME uses a variety of eruption and environmental parameters as input and returns ash and radioactive waste concentrations at select locations on the ground surface as output. This code is called by GoldSim.

CWD - This code calculates cumulative probability distributions for the occurrence and size of manufacturing defects in the closure welds of the waste packages given the non-detection probability and the fraction of defects to be considered. The calculations are based on the abstraction of defect density and size distributions. This code is called by GoldSim.

FEHM - This code is a Finite Element, Heat and Mass transfer code utilized for flow and transport calculations. External to GoldSim, the code will be used to develop saturated-zone breakthrough curves at various distances from the proposed repository. Internal to GoldSim, at each timestep in the TSPA model, FEHM reads a set of pre-generated flow fields and performs the unsaturated zone particle transportation simulation. GoldSim uses the results of the Unsaturated Zone (UZ) particle transport simulation as input for the saturated zone model.

GVP - The Gaussian Variance Partitioning software was developed to incorporate measurement uncertainty and corrosion rate variability into the calculations of waste package degradation. To assess waste package failure distributions over time in the repository, only a fraction of the total variance is considered to be due to variability in the waste package degradation simulations. Gaussian Variance Partitioning is applied to separate the contributions of uncertainty and variability from the composite distribution. The approach to uncertainty and variability in the waste package degradation modeling may be modified for TSPA-LA.

MKTable - This code processes data used in simulating long-term degradation of the waste package in the repository. This code is called by GoldSim.

Patch Fail Lag - The software reads in the waste package failure curve, waste package failed patch curve, and drip shield failed patch curve. It then determines the time at which the first waste package fails. The waste package and drip shield failed patch curves are then shifted backwards in time by the time of first waste package failure. The software passes the shifted curves back into the GoldSim TSPA Model.

SCCD - This code was developed to model stress corrosion crack initiation and then propagation in the closure welds of manufacturing defects and incipient weld cracks. A reference table stress intensity factor as a function of crack depth is modified by SCCD and used as input into WAPDEG. This code is called by WAPDEG during its operation within GoldSim. The resulting waste package failure histories are then returned to GoldSim.

SEEPAGEDLLMK2_UU - This code calculates the seepage into the drifts across the repository. Spatial variability and uncertainty are accounted for in the seepage calculation.

SOILEXP - This code calculates the cumulative soil removal factor used to calculate radionuclide concentration in volcanic ash deposits. The code receives input from GoldSim, calculates the cumulative soil removal for the time interval being simulated and passes the result back to GoldSim for use in dose calculations. This code is used only in eruptive modeling case calculations.

SZ_Convolute - This code calculates the mass flux response curves during the time interval immediately after a climate change at the saturated zone (SZ) outflow boundary based on the saturated zone generic response curves and unsaturated zone radionuclide source terms for the analyses.

WAPDEG - This code was developed to simulate waste package degradation using a stochastic approach. The WAPDEG DLL evaluates and applies initiation thresholds of various corrosion and other degradation processes as a function of time-dependent exposure conditions. The penetration rate of active degradation process as a function of time is also evaluated. WAPDEG generates output of time histories of failures and subsequent degradation for waste packages.

2.2 MODEL CONFIGURATION MANAGEMENT

The proposed Yucca Mountain repository is comprised of a complex system of engineered and natural barriers. To better understand these barriers, detailed external process models have been developed to evaluate the overall performance of the repository. Software codes are used to implement these models. The specific information on these codes and a detailed model description is contained in the individual process model documentation. The TSPA department uses the key results of this documentation to model the repository system. The system is represented in the TSPA in a comprehensive integrated model implemented using the GoldSim software code. All of the submodels implemented in GoldSim as well as the external process models will be developed and validated in accordance with AP-SIII.10Q, *Models*. Output files from process level submodels that are required as GoldSim input files will be submitted to the Technical Data Management System (TDMS) per AP-SIII.3Q, *Submittal and Incorporation of Data to the Technical Data Management System*, and are uniquely identified with a data tracking number (DTN). The development of the TSPA-LA model will also be controlled in GoldSim. During development, the GoldSim model file and its external files will be stored on a controlled directory. Any proposed changes or modifications to the controlled model file will be reviewed and approved by the TSPA Department Manager prior to the change being implemented. All changes to the model will be checked. For specific details on the model development, model checking and model change control, see Section 6, Control of the TSPA-LA Model. Figure 2.2-1 provides a high-level view of the model development and analysis process.

2.3 CONFIGURATION MANAGEMENT OF TSPA MODEL INPUTS

The TSPA-LA model is a computer model that will integrate the process models and abstractions developed for the proposed repository. All parameters implemented in the model will be controlled, captured and submitted to the TDMS as part of the TSPA-LA model file. Figure 2.3-1 provides an overview of the TSPA-LA model information flow from initial data development, to external process models, to the implementation in GoldSim, and back to the TDMS. The qualification status of all the inputs can be found in the TDMS database. Again, the starting point and basis for the TSPA-LA model is the TSPA-FEIS model. The TSPA-FEIS model is not a validated model, and contains both "Q" and "non-Q" inputs. Each TSPA-FEIS input file and the file description is listed in Table 2.3-1. This table provides the initial input files as a starting point for the TSPA-LA model, but these files are expected to be modified prior to finalizing the TSPA-LA model. The TSPA-LA model will be validated; therefore, prior to finalizing the TSPA-LA model, all the parameters will be controlled and the software used in the model will be qualified.

Table 2.3-1. TSPA-FEIS Input Files (WAPDEG, FEHM, Seepage, SZ_Convolute)

WAPDEG Files	Size (bytes)	Date	Description
WD4DLL.wap	335	04/06/01	List of input files to WAPDEG dll
WDgA22SR00.cdf	12,524	05/12/00	Corrosion rate for Alloy 22
WDgA22x0p5.cdf	12,524	05/12/00	Corrosion rate for Alloy 22*0.5
WDgA22x2p5.cdf	12,524	05/12/00	Corrosion rate for Alloy 22*2.5
WDgTi7SR00.cdf	12,526	05/24/00	Corrosion rate for titanium
WDhist.inp	1,002	05/17/01	List of inputs Make_History_WAP
WDKlinM.fil	1,436	01/14/00	Stress intensity factor versus depth profiles for middle lid
WDKlinO.fil	1,439	01/14/00	Stress intensity factor versus depth for outer lid
WDRHcrit.fil	411	02/24/00	Critical threshold RH versus exposure temperature
csnf_HTOM_high_bin2.ou	172,601	05/17/01	CSNF, HTOM, high infiltration, bin 2
csnf_HTOM_high_bin3.ou	822,551	05/17/01	CSNF, HTOM, high infiltration, bin 3
csnf_HTOM_high_bin4.ou	10,067,228	05/17/01	CSNF, HTOM, high infiltration, bin 4
csnf_HTOM_high_bin5.ou	5,471,675	05/17/01	CSNF, HTOM, high infiltration, bin 5
csnf_HTOM_low_bin1.ou	9,287,822	05/17/01	CSNF, HTOM, low infiltration, bin 1
csnf_HTOM_low_bin2.ou	5,249,759	05/17/01	CSNF, HTOM, low infiltration, bin 2
csnf_HTOM_mean_bin2.ou	916,541	05/17/01	CSNF, HTOM, medium infiltration, bin 2
csnf_HTOM_mean_bin3.ou	4,584,788	05/17/01	CSNF, HTOM, medium infiltration, bin 3
csnf_HTOM_mean_bin4.ou	10,661,318	05/17/01	CSNF, HTOM, medium infiltration, bin 4
csnf_LTOM_high_bin2.ou	167,813	07/26/01	CSNF, LTOM, high infiltration, bin 2
csnf_LTOM_high_bin3.ou	2,851,669	07/26/01	CSNF, LTOM, high infiltration, bin 3
csnf_LTOM_high_bin4.ou	10,064,532	07/26/01	CSNF, LTOM, high infiltration, bin 4
csnf_LTOM_high_bin5.ou	5,176,080	07/26/01	CSNF, LTOM, high infiltration, bin 5
csnf_LTOM_low_bin1.ou	12,772,351	07/26/01	CSNF, LTOM, low infiltration, bin 1
csnf_LTOM_low_bin2.ou	5,487,599	07/26/01	CSNF, LTOM, low infiltration, bin 2
csnf_LTOM_mean_bin2.ou	2,899,595	07/26/01	CSNF, LTOM, medium infiltration, bin 2
csnf_LTOM_mean_bin3.ou	5,176,080	07/26/01	CSNF, LTOM, medium infiltration, bin 3
csnf_LTOM_mean_bin4.ou	10,184,347	07/26/01	CSNF, LTOM, medium infiltration, bin 4
hlw_HTOM_high_bin2.ou	179,783	05/17/01	HLW, HTOM, high infiltration, bin 2

Table 2.3-1. TSPA-FEIS Input Files (WAPDEG, FEHM, Seepage, SZ_Convolute) (Continued)

WAPDEG Files	Size (bytes)	Date	Description
hlw_HTOM_high_bin3.ou	845,161	05/17/01	HLW, HTOM, high infiltration, bin 3
hlw_HTOM_high_bin4.ou	10,294,658	05/17/01	HLW, HTOM, high infiltration, bin 4
hlw_HTOM_high_bin5.ou	5,639,255	05/17/01	HLW, HTOM, high infiltration, bin 5
hlw_HTOM_low_bin1.ou	9,625,376	05/17/01	HLW, HTOM, low infiltration, bin 1
hlw_HTOM_low_bin2.ou	5,428,245	05/17/01	HLW, HTOM, low infiltration, bin 2
hlw_HTOM_mean_bin2.ou	943,407	05/17/01	HLW, HTOM, medium infiltration, bin 2
hlw_HTOM_mean_bin3.ou	4,684,804	05/17/01	HLW, HTOM, medium infiltration, bin 3
hlw_HTOM_mean_bin4.ou	10,934,500	05/17/01	HLW, HTOM, medium infiltration, bin 4
hlw_LTOM_high_bin2.ou	167,813	07/26/01	HLW, LTOM, high infiltration, bin 2
hlw_LTOM_high_bin3.ou	2,851,669	07/26/01	HLW, LTOM, high infiltration, bin 3
hlw_LTOM_high_bin4.ou	10,064,532	07/26/01	HLW, LTOM, high infiltration, bin 4
hlw_LTOM_high_bin5.ou	5,176,080	07/26/01	HLW, LTOM, high infiltration, bin 5
hlw_LTOM_low_bin1.ou	12,772,351	07/26/01	HLW, LTOM, low infiltration, bin 1
hlw_LTOM_low_bin2.ou	5,487,599	07/26/01	HLW, LTOM, low infiltration, bin 2
hlw_LTOM_mean_bin2.ou	2,899,595	07/26/01	HLW, LTOM, medium infiltration, bin 2
hlw_LTOM_mean_bin3.ou	5,176,080	07/26/01	HLW, LTOM, medium infiltration, bin 3
hlw_LTOM_mean_bin4.ou	10,184,347	07/26/01	HLW, LTOM, medium infiltration, bin 4
FEHM Files	**Size (bytes)**	**Date**	**Description**
afm_pch1.dpdp	3,715	01/05/00	fracture porosity & half-spacing file
bf2.txt	77	03/13/00	colloid size distribution file
bf3.txt	77	03/13/00	colloid size distribution file
ch1.txt,	77	03/13/00	colloid size distribution file
ch6.txt,	77	03/13/00	colloid size distribution file
chv.txt,	77	03/13/00	colloid size distribution file
chz.txt,	77	03/13/00	colloid size distribution file
fehmn.files	291	02/15/00	input control file
fehmn.gold	1,278	05/04/01	commands for FEHM .bat files
ff0100.ini,	15,937,540	10/11/99	flow field file
ff0200.ini,	15,937,540	10/11/99	flow field file
ff0300.ini	15,937,540	10/11/99	flow field file
ff1100.ini,	15,938,094	10/14/99	flow field file
ff1200.ini,	15,938,094	10/14/99	flow field file
ff1300.ini	15,938,094	10/14/99	flow field file
ff2100.ini,	15,938,094	10/14/99	flow field file
ff2200.ini,	15,938,094	10/14/99	flow field file
ff2300.ini	15,938,094	10/14/99	flow field file
ff3000.ini	15,938,094	09/08/00	flow field file
ff3500.ini	15,938,094	09/08/00	flow field file
ff4000.ini	15,938,094	09/08/00	flow field file
ff5000.ini	15,938,094	09/08/00	flow field file
fm_pchm1.dat	1,630	07/29/00	Input file containing time step ptrk info
fm_pchm1_1E5.dat	1,630	07/29/00	FEHM input files for run durations
fm_pchm1_1E6.dat	1,630	07/29/00	FEHM input files for run durations
fm_pchm1_2E4.dat	1,630	07/29/00	FEHM input files for run durations
fm_pchm1_3E5.dat	1,630	07/29/00	FEHM input files for run durations
fm_pchm1.grid	2,335,583	01/04/00	grid file
fm_pchm1.stor	29,301,805	01/04/00	stiffness matrix file
fm_pchm1.zone	980,781	01/04/00	zone file
fm_pchm1.zone2	1,082,426	03/03/00	zone file
fm_pchm1.zone2.0100	1,082,424	03/03/00	zone file
fm_pchm1.zone2.0200	1,082,426	03/03/00	zone file
fm_pchm1.zone2.0300	1,082,424	03/03/00	zone file
pch1.rock	3,349	01/04/00	rock properties file
pp1.txt	77	03/13/00	colloid size distribution file
pp2.txt	77	03/13/00	colloid size distribution file

Table 2.3-1. TSPA-FEIS Input Files (WAPDEG, FEHM, Seepage, SZ_Convolute) (Continued)

pp3.txt	77	03/13/00	colloid size distribution file

Table 2.3-1. TSPA-FEIS Input Files (WAPDEG, FEHM, Seepage, SZ_Convolute) (Continued)

FEHM Files	Size (bytes)	Date	Description
pp4.txt	77	03/13/00	colloid size distribution file
ptrk.multrlz	2,030,063	08/22/00	particle tracking file
ptrk.multrlz.0100	2,030,069	08/22/00	particle tracking file for multiple realizations
ptrk.multrlz.0200	2,030,063	08/22/00	Particle tracking file for multiple realizations
ptrk.multrlz.0300	2,030,060	04/12/01	Particle tracking file for multiple realizations
tsw4.txt	77	03/13/00	colloid size distribution file
tsw5.txt	77	03/13/00	colloid size distribution file
tsw6.txt	77	03/13/00	colloid size distribution file
tsw7.txt	77	03/13/00	colloid size distribution file
tsw8.txt	77	03/13/00	colloid size distribution file
tsw9.txt	77	03/13/00	colloid size distribution file
UZ_Params_Multi_.sr	176,012	05/10/00	UZ sampled parameters file
UZ_Params_Multi_1000rlz.sr	176,012	05/10/00	UZ sampled parameters file for multiple realizations
UZ_Params_Multi_100rlz.sr	176,012	05/10/00	UZ sampled parameters file for multiple realizations
UZ_Params_Multi_3000rlz.sr	176,012	05/10/00	UZ sampled parameters file for multiple realizations
UZ_Params_Multi_300rlz.sr	176,012	05/10/00	UZ sampled parameters file for multiple realizations
UZ_Params_Multi_5000rlz.sr	176,012	05/10/00	UZ sampled parameters file for multiple realizations
Seepage Files	**Size (bytes)**	**Date**	**Description**
CSNF_HT_high_pf_bin2.txt	103,535	05/14/01	CSNF, HTOM, high infiltration, bin 2
CSNF_HT_high_pf_bin3.txt	517,319	05/14/01	CSNF, HTOM, high infiltration, bin 3
CSNF_HT_high_pf_bin4.txt	6,059,069	05/14/01	CSNF, HTOM, high infiltration, bin 4
CSNF_HT_high_pf_bin5.txt	3,236,471	05/14/01	CSNF, HTOM, high infiltration, bin 5
CSNF_HT_low_pf_bin1.txt	6,384,185	05/14/01	CSNF, HTOM, low infiltration, bin 1
CSNF_HT_low_pf_bin2.txt	3,532,031	05/14/01	CSNF, HTOM, low infiltration, bin 2
CSNF_HT_mean_pf_bin2.txt	576,431	05/14/01	CSNF, HTOM, medium infiltration, bin 2
CSNF_HT_mean_pf_bin3.txt	2,867,021	05/14/01	CSNF, HTOM, medium infiltration, bin 3
CSNF_HT_mean_pf_bin4.txt	6,472,853	05/14/01	CSNF, HTOM, medium infiltration, bin 4
CSNF_LT2_high_pf_bin2.txt	103,535	07/24/01	CSNF, LTOM, high infiltration, bin 2
CSNF_LT2_high_pf_bin3.txt	1,758,671	07/24/01	CSNF, LTOM, high infiltration, bin 3
CSNF_LT2_high_pf_bin4.txt	6,206,849	07/24/01	CSNF, LTOM, high infiltration, bin 4
CSNF_LT2_high_pf_bin5.txt	3,192,137	07/24/01	CSNF, LTOM, high infiltration, bin 5
CSNF_LT2_low_pf_bin1.txt	7,876,763	07/24/01	CSNF, LTOM, low infiltration, bin 1
CSNF_LT2_low_pf_bin2.txt	3,384,251	07/24/01	CSNF, LTOM, low infiltration, bin 2
CSNF_LT2_mean_pf_bin2.txt	1,788,227	07/24/01	CSNF, LTOM, medium infiltration, bin 2
CSNF_LT2_mean_pf_bin3.txt	3,192,137	07/24/01	CSNF, LTOM, medium infiltration, bin 3
CSNF_LT2_mean_pf_bin4.txt	6,280,739	07/24/01	CSNF, LTOM, medium infiltration, bin 4
HLW_HT_high_pf_bin2.txt	103,535	05/14/01	HLW, HTOM, high infiltration, bin 2
HLW_HT_high_pf_bin3.txt	517,319	05/14/01	HLW, HTOM, high infiltration, bin 3
HLW_HT_high_pf_bin4.txt	6,059,069	05/14/01	HLW, HTOM, high infiltration, bin 4
HLW_HT_high_pf_bin5.txt	3,236,471	05/14/01	HLW, HTOM, high infiltration, bin 5
HLW_HT_low_pf_bin1.txt	6,384,185	05/14/01	HLW, HTOM, low infiltration, bin 1
HLW_HT_low_pf_bin2.txt	3,532,031	05/14/01	HLW, HTOM, low infiltration, bin 2
HLW_HT_mean_pf_bin2.txt	576,431	05/14/01	HLW, HTOM, medium infiltration, bin 2
HLW_HT_mean_pf_bin3.txt	2,867,021	05/14/01	HLW, HTOM, medium infiltration, bin 3
HLW_HT_mean_pf_bin4.txt	6,472,853	05/14/01	HLW, HTOM, medium infiltration, bin 4
HLW_LT2_high_pf_bin2.txt	103,535	07/24/01	HLW, LTOM, high infiltration, bin 2
HLW_LT2_high_pf_bin3.txt	1,758,671	07/24/01	HLW, LTOM, high infiltration, bin 3

Table 2.3-1. TSPA-FEIS Input Files (WAPDEG, FEHM, Seepage, SZ_Convolute) (Continued)

HLW_LT2_high_pf_bin4.txt	6,206,849	07/24/01	HLW, LTOM, high infiltration, bin 4
HLW_LT2_high_pf_bin5.txt	3,192,137	07/24/01	HLW, LTOM, high infiltration, bin 5
HLW_LT2_low_pf_bin1.txt	7,876,763	07/24/01	HLW, LTOM, low infiltration, bin 1
HLW_LT2_low_pf_bin2.txt	3,384,251	07/24/01	HLW, LTOM, low infiltration, bin 2
Seepage Files	**Size (bytes)**	**Date**	**Description**
HLW_LT2_mean_pf_bin2.txt	1,788,227	07/24/01	HLW, LTOM, medium infiltration, bin 2
HLW_LT2_mean_pf_bin3.txt	3,192,137	07/24/01	HLW, LTOM, medium infiltration, bin 3
HLW_LT2_mean_pf_bin4.txt	6,280,739	07/24/01	HLW, LTOM, medium infiltration, bin 4
master_bf.in	543	05/03/01	input control file
master_nbf.in	561	07/24/01	input control file
SeepFlowMean.dat	439	04/02/01	mean seepage flow distribution data
SeepFlowSD.dat	425	04/02/01	seepage flow S.D. distribution data
SeepFrac.dat	404	04/02/01	seepage fraction distribution data
SZ_Convolute Files	**Size/bytes**	**Date**	**Description**
SZ_01_01	3,604,849	07/25/01	RN Type 1, Region 1 BTCs
SZ_01_02	3,604,849	07/25/01	RN Type 1, Region 2 BTCs
SZ_01_03	3,604,849	07/25/01	RN Type 1, Region 3 BTCs
SZ_01_04	3,604,849	07/25/01	RN Type 1, Region 4 BTCs
SZ_02_01	3,604,849	07/25/01	RN Type 2, Region 1 BTCs
SZ_02_02	3,604,849	07/25/01	RN Type 2, Region 2 BTCs
SZ_02_03	3,604,849	07/25/01	RN Type 2, Region 3 BTCs
SZ_02_04	3,604,849	07/25/01	RN Type 2, Region 4 BTCs
SZ_03_01	3,604,849	07/25/01	RN Type 3, Region 1 BTCs
SZ_03_02	3,604,849	07/25/01	RN Type 3, Region 2 BTCs
SZ_03_03	3,604,849	07/25/01	RN Type 3, Region 3 BTCs
SZ_03_04	3,604,849	07/25/01	RN Type 3, Region 4 BTCs
SZ_04_01	3,604,849	07/25/01	RN Type 4, Region 1 BTCs
SZ_04_02	3,604,849	07/25/01	RN Type 4, Region 2 BTCs
SZ_04_03	3,604,849	07/25/01	RN Type 4, Region 3 BTCs
SZ_04_04	3,604,849	07/25/01	RN Type 4, Region 4 BTCs
SZ_05_01	3,604,849	07/25/01	RN Type 5, Region 1 BTCs
SZ_05_02	3,604,849	07/25/01	RN Type 5, Region 2 BTCs
SZ_05_03	3,604,849	07/25/01	RN Type 5, Region 3 BTCs
SZ_05_04	3,604,849	07/25/01	RN Type 5, Region 4 BTCs
SZ_06_01	3,604,849	07/25/01	RN Type 6, Region 1 BTCs
SZ_06_02	3,604,849	07/25/01	RN Type 6, Region 2 BTCs
SZ_06_03	3,604,849	07/25/01	RN Type 6, Region 3 BTCs
SZ_06_04	3,604,849	07/25/01	RN Type 6, Region 4 BTCs
SZ_07_01	3,604,849	07/25/01	RN Type 7, Region 1 BTCs
SZ_07_02	3,604,849	07/25/01	RN Type 7, Region 2 BTCs
SZ_07_03	3,604,849	07/25/01	RN Type 7, Region 3 BTCs
SZ_07_04	3,604,849	07/25/01	RN Type 7, Region 4 BTCs
SZ_08_01	3,604,849	07/25/01	RN Type 8, Region 1 BTCs
SZ_08_02	3,604,849	07/25/01	RN Type 8, Region 2 BTCs
SZ_08_03	3,604,849	07/25/01	RN Type 8, Region 3 BTCs
SZ_08_04	3,604,849	07/25/01	RN Type 8, Region 4 BTCs
SZ_Convolute2.dat	432	06/02/01	input file

Notes: Bin "x" denotes one of the five infiltration bins in the TSPA model. For TSPA-LA, the appropriate files will all be submitted to TDMS. See acronym list (Appendix A) for other acronym definitions.

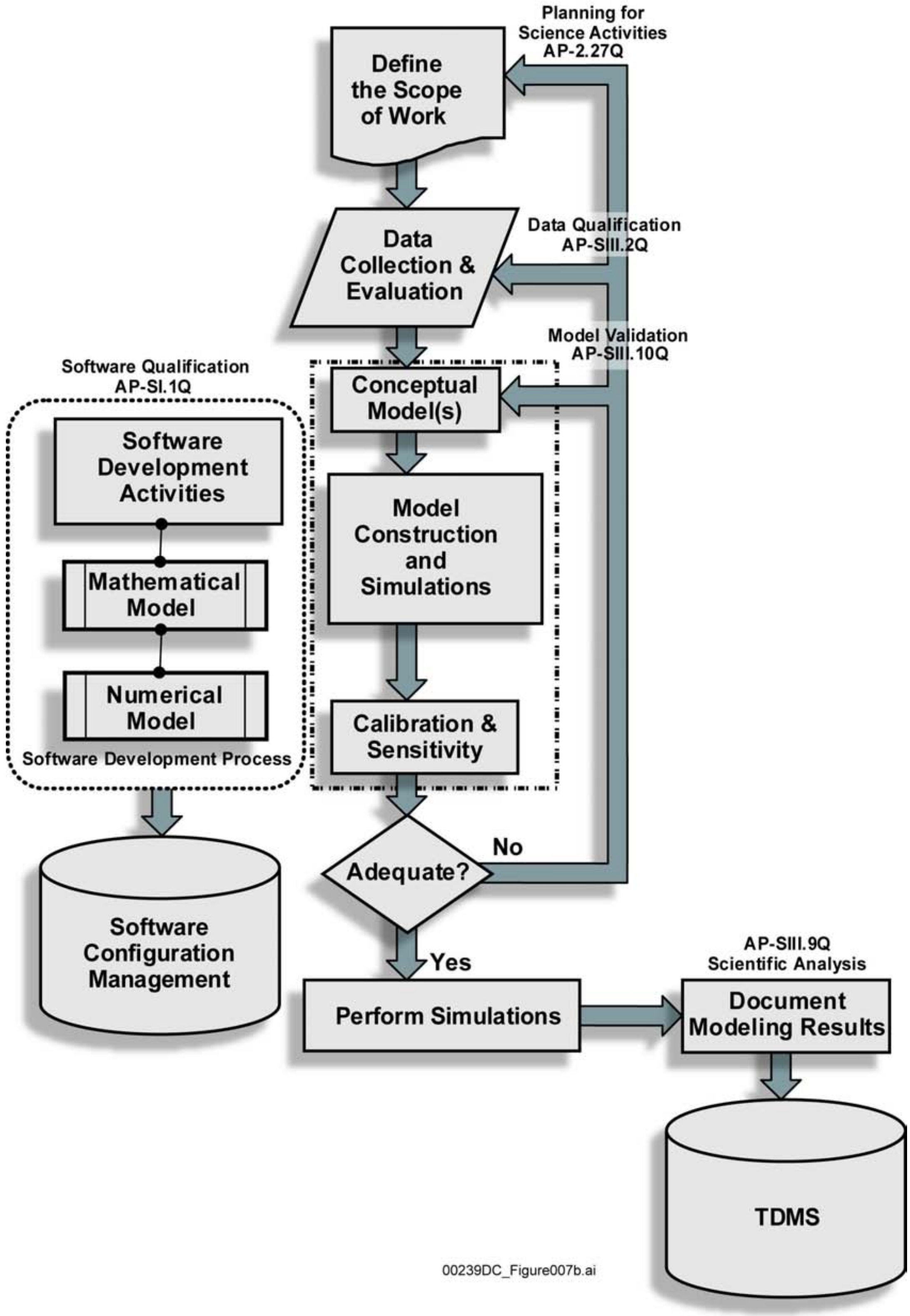


Figure 2.2-1. General Overview of the TSPA-LA Model Development and Analysis Process

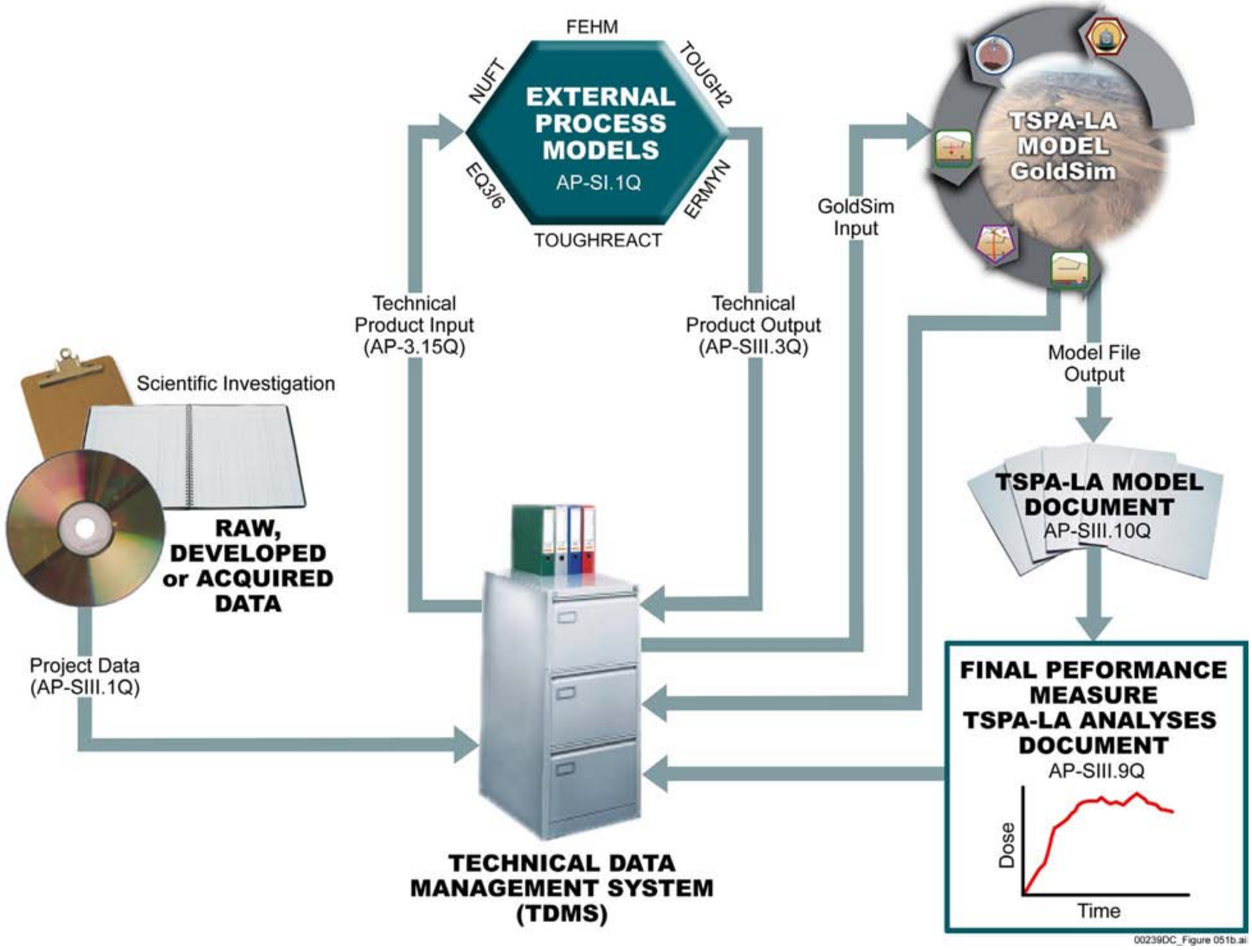


Figure 2.3-1 Overview of the TSPA-LA Model Information Flow

3. PROCESSES FOR TSPA-LA

A major licensing requirement for the disposal of high-level radioactive waste at the proposed Yucca Mountain geologic repository is the evaluation of postclosure performance. The NRC, in their regulation, 10 CFR Part 63, requires that a performance assessment (PA) analysis be performed for this evaluation. The definition of a performance assessment, as defined by the NRC in 10 CFR 63.2, was provided in Section 1.3.

The EPA and NRC, in their regulations (40 CFR Part 197 and 10 CFR Part 63, respectively) specifically acknowledge that uncertainty in dose (item 3 in the definition of a performance assessment, from 10 CFR 63.2) is a key issue and call for including uncertainty in order to develop a "reasonable expectation" of compliance. Reasonable expectation is defined in 10 CFR 63.304 as:

> "*Reasonable expectation* means that the Commission is satisfied that compliance will be achieved based upon the full record before it. Characteristics of reasonable expectation include that it:
>
> (1) Requires less than absolute proof because absolute proof is impossible to attain for disposal due to the uncertainty of projecting long-term performance;
> (2) Accounts for the inherently greater uncertainties in making long-term projections of the performance of the Yucca Mountain disposal system;
> (3) Does not exclude important parameters from assessments and analyses simply because they are difficult to precisely quantify to a high degree of confidence; and
> (4) Focuses performance assessments and analyses on the full range of defensible and reasonable parameter distributions rather than only upon extreme physical situations and parameter values."

Hence, identifying, categorizing, quantifying, evaluating, and documenting uncertainties (as discussed in Sections 3.2 through 3.5) are important tasks of a performance assessment (hereafter referred to as a total system performance assessment [TSPA] to emphasize the inclusion of all subsystems of the Yucca Mountain disposal system). Much progress in accomplishing these tasks was made in performing the *FY 01 Supplemental Science and Performance Analyses, Volume 1: Scientific Bases and Analyses* (BSC 2001 [155950]) and *FY01 Supplemental Science and Performance Analyses, Volume 2: Performance Analyses* (BSC 2001 [154659]), collectively referred to as the SSPA. Performing these tasks in a consistent manner is also important for regulatory review. Processes for building upon the progress in the SSPA and providing additional consistency for TSPA-LA have been developed in *Guidelines for Developing and Documenting Alternative Conceptual Models, Model Abstractions, and Parameter Uncertainty in the Total System Performance Assessment for the License Application* (BSC 2002 [158794]) (referred to as the *Guidelines Document* hereafter) and are summarized in this section.

Section 3.1 introduces key terms and the team concept that will be used to treat uncertainty consistently in TSPA-LA. The concepts of aleatory and epistemic uncertainty are discussed. As repeated often in radioactive waste disposal literature, the three major sources of uncertainty in analyses of geologic disposal systems are uncertainty in (1) completeness (i.e., uncertainty in capturing all applicable features, events, and processes (FEPs) of item 1 of the PA definition in Section 1.3); (2) model form (i.e., uncertainty about the hypotheses and appropriate model definition in evaluating the dose and calculating the probability of FEP occurrence); and (3) parameters (i.e., uncertainty in the appropriate parameter values to use in the selected models for consequence and probability).

Section 3.2 describes the current status of FEPs and enhancements planned for the TSPA-LA as outlined in *The Enhanced Plan for Features, Events, and Processes (FEPs) at Yucca Mountain* (BSC 2002 [158966]) (referred to as *Enhanced FEPs Plan* hereafter). Sections 3.3 and 3.4 discuss the basic processes established in the treatment of model form uncertainty (divided further into alternative conceptual models and model abstractions). Section 3.5 discusses parameter uncertainty.

3.1 UNCERTAINTY

By way of introduction, 10 CFR 63.114 states:

> "Any performance assessment used to demonstrate compliance with 10 CFR 63.114 must:…(b) Account for uncertainties and variabilities in parameter values and provide for the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment."

The uncertainty referred to in this part of the regulation concerns the lack of knowledge in parameter values, which is also called epistemic uncertainty. Another type of uncertainty is addressed in the regulation, whereby 10 CFR 63.2 states:

> "Performance assessment means an analysis that: … (3) Estimates the dose incurred by the reasonably maximally exposed individual, including the associated uncertainties, as a result of releases caused by all significant features, events, processes, and sequences of events and processes, weighted by their probability of occurrence."

The uncertainty referred to in this part of the regulation, associated with chance occurrences, is also called aleatory uncertainty. This section distinguishes between the two types of uncertainty mentioned (aleatory and epistemic) and introduces the team approach to treating uncertainty such that the performance assessment consistently and adequately provides the technical basis for parameter ranges and distributions.

3.1.1 Aleatory and Epistemic Uncertainty

A TSPA for a radioactive waste disposal facility is a complex undertaking, requiring large amounts of information and a variety of mathematical models. Full documentation of a TSPA can require thousands of pages. Yet, at a conceptual level, the computational implementation of a TSPA can be viewed as involving the answers to four basic questions (Helton 1996 [107823], Kaplan and Garrick 1981 [100557]). First, "What occurrences can take place at the facility under consideration?" From the answer to this question follows the second question, "How likely are these occurrences to take place?" and the third question, "What are the consequences of individual occurrences?" Finally, the fourth question asks, "How much confidence exists in the answers to the first three questions?"

Standing above these questions in a TSPA is a process referred to as the screening of features, events, and processes (FEPs). It is from this screening, which is initially informal and ultimately very structured, that the information emerges that is needed to answer the preceding questions. In particular, the FEPs process gathers, assesses, and winnows the information that ultimately leads to the formal computational structure and associated calculations that provide the quantitative answers to the last three questions (i.e., probabilities, doses, uncertainty assessments).

The first and second questions involve the occurrence and likelihood of events that take place in the future. Such occurrences are assumed to have a random character in the sense that their likelihood of taking place over various intervals of time can be estimated, but it is not possible to determine whether or not they will actually occur. Such uncertainty is often given the designation "aleatory." Examples of aleatory uncertainty include the occurrence of seismic events, igneous events, and particular spatial patterns of corrosion. Alternative designations for aleatory uncertainty include Type A, stochastic, irreducible, and objective uncertainty. In concept and within the resource limitations of a particular analysis, aleatory uncertainty can be better characterized through additional study but cannot be removed by such study.

The third question relates to the models used to analyze physical behavior of the system under consideration, as well as the determination of the consequences of the various occurrences that could take place in the system. Such models can be viewed as functions that predict consequences for particular occurrences or sequences of occurrences. Such models are often quite complex (e.g., systems of nonlinear ordinary or partial differential equations). Models that are constructed by combining many individual models are common in performance assessment for radioactive waste disposal. Often, much of the human and computational resources expended in a large performance assessment are devoted to the development, parameterization, and numerical evaluation of models used to predict the consequences associated with particular occurrences (e.g., undisturbed conditions, human intrusion, seismic events, igneous events, …).

The fourth question relates to a type of uncertainty that is distinct from aleatory uncertainty. This second type of uncertainty is involved with the degree of appropriateness or validity that can be assigned to the assumptions and quantities used in the TSPA model. Such uncertainty is often given the designation "epistemic." Epistemic uncertainty arises from a lack of knowledge about a parameter because the data are limited or because there are alternative interpretations of the available data. The parameter is not variable because of an intrinsic characteristic of the entity under study but because an analyst does not know what the precise value of the parameter should be. For example, there is substantial epistemic uncertainty in many quantities used in TSPA for the proposed repository (e.g., solubilities, distribution coefficients, permeabilities). Often, quantities used in performance assessments are expected values over spatial or temporal variation, with significant epistemic uncertainty existing with respect to the appropriate values to use for these expected values. Further, there can also be epistemic uncertainty in quantities used to characterize aleatory uncertainty (e.g., rates at which igneous and seismic events occur). This type of inexactness is also called Type B, state of knowledge, reducible, and subjective uncertainty. Epistemic refers to the state of knowledge about a parameter. The state of knowledge about the exact value of the parameter can increase through testing and data collection such that the uncertainty is "reducible." Epistemic uncertainty also includes model uncertainty (i.e., what is the appropriate model or model structure to use in a particular modeling context?).

Most performance assessments use probability to characterize both aleatory and epistemic uncertainty (Helton et al. 2000 [159062]; SNL 1996 [126532]; PLG 1983 [107813]; PLG 1983 [148063]; PLG 1982 [107812]; NRC 1990 [107798]). Indeed, the use of probability to characterize both aleatory and epistemic uncertainty can be traced to the beginnings of the formal development of probability in the late seventeenth century (Bernstein 1996 [105742]; Hacking 1975 [107512]; Shafer 1978 [159070]). Other representations of uncertainty exist (e.g., evidence theory, possibility theory, fuzzy set theory) but are not widely used in performance assessment and will not be discussed here. Consistent with other performance assessments for complex systems, the performance assessment for the proposed repository uses probability to characterize both aleatory and epistemic uncertainty.

Distinguishing between these two types of uncertainty is not necessary for the estimation of mean dose, but is important in many instances to understand the results and how the uncertainties in dose might be better characterized (or possibly reduced) by the collection of more data (Apostolakis 1990 [107506]; Barnett and O'Hagan 1997 [158964]; Cullen and Frey 1999 [107797]; Helton 1994 [107739]; Helton 1997 [107496]; Helton and Burmaster 1996 [107498]; Parry and Winter 1981 [159059]; Paté-Cornell 1996 [107499]). The desire to maintain a separation between aleatory and epistemic uncertainty affects the design of the analyses (e.g., separate analysis of volcanic disruption and no volcanic disruption). It may also affect the design of individual model components (e.g., the model component for corrosion of the waste package). Because of this influence, choices will be made during TSPA-LA development concerning which uncertainties will be treated as aleatory and which will be treated as epistemic in developing submodels or components of the TSPA and designing the TSPA analysis (e.g., selecting scenarios to propagate through the TSPA system model). If the TSPA does not maintain a separation between aleatory and epistemic uncertainty for a specific parameter, then the total uncertainty is expressed as a combined distribution. The description of parameter uncertainty of all the remaining parameters (designated as either epistemic parameters or combined epistemic/aleatory parameters) is discussed in Section 3.5.

3.1.2 Team Approach for Treating Uncertainty in Model Form and Parameters

The TSPA-LA must integrate information from many sources and document the uncertainty from these numerous sources. An external review of TSPA-SR (*Evaluation of Uncertainty Treatment in the Technical Documents Supporting TSPA-SR* (YMP 2001 [155343]) found numerous examples of parameters where the documentation adequately explained the various sources of uncertainty (e.g., measurement error or experiment representativeness); however, in other situations this documentation was lacking. To maintain consistency in the interface with other organizations as well as consistency in the integration and documentation of the technical basis for parameter ranges and distributions, the Performance Assessment Strategy and Scope group has established a team leader in parameter uncertainty, the Parameter Team Lead (PTL), and a team leader for model form uncertainty, the Abstraction Team Lead (ATL). A separate team is formed for individual uncertain parameters or groups of related uncertain parameters. Each team has two additional members, (1) a Subject Matter Expert (SME) from the appropriate department, who is most knowledgeable about individual underlying process models and their uncertain parameters, and (2) a TSPA analyst from the TSPA Department, who is knowledgeable about the use of the parameter(s) in the TSPA. The SME and TSPA analyst may be different for each team, and each model may therefore have its own team. The ATL (or PTL) will be a common member on all of the teams. These primary team members are supported by various other personnel. Sections 3.3 through 3.5 provide more details as they pertain to model form and parameter uncertainty.

3.2 FEATURES, EVENTS, AND PROCESSES

The development of a comprehensive list of FEPs potentially relevant to the postclosure performance of the proposed repository is an ongoing, iterative process based on site-specific information, design, and regulations. Features are physical, chemical, thermal, or temporal characteristics of the site or repository system. Examples of features are the waste package and fracture systems. Processes are typically phenomena and activities that have gradual, continuous interactions with the repository system or subsystem. An example of a process is percolation of water into the unsaturated rock above the repository. Events may be interrelated with processes, but in general, events are discrete occurrences. An example of an event is volcanism.

For TSPA-SR, FEPs analysis and subsequent scenario development followed a five-step process:

1. Identification of FEPs
2. Classification of FEPs
3. Screening of FEPs
4. Formation of Scenario Classes
5. Screening of Scenario Classes

These five steps are further described in Section 2.1.1.1 of the *Total System Performance Assessment for the Site Recommendation* (CRWMS M&O 2000 [153246]). Specific details of the initial FEP analysis (identification, classification, and screening) for TSPA-SR were documented in Sections 2 through 4 of *The Development of Information Catalogued in REV 00 of the YMP FEP Database* (Freeze et al. 2001 [154365]) (referred to as *FEP Database Report* hereafter). A series of FEP Analysis Model Reports (AMRs), listed in Table 3.2-1, were developed to document the technical basis for inclusion or exclusion of FEPs from TSPA-SR. This table presents the latest revision, which may postdate the TSPA-SR. The relevant information in these FEP AMRs was subsequently transferred to a Yucca Mountain Project

(YMP) FEP Database (Freeze et al. 2001 [154365], Section 5) to provide a navigational tool for reviewing and analyzing FEPs.

Table 3.2-1. FEP AMRs Documenting Screening Information in Support of TSPA-SR

Subject Area	Reference
Unsaturated Zone Flow and Transport	(BSC 2001 [154826])
Saturated Zone Flow and Transport	(CRWMS M&O 2001 [153931])
Biosphere	(BSC 2001 [153921])
Disruptive Events	(CRWMS M&O 2000 [151553])
Waste Package Degradation	(CRWMS M&O 2001 [153937])
Waste Form Degradation - Miscellaneous - Cladding - Colloid	 (CRWMS M&O 2001 [153938]) (CRWMS M&O 2000 [153947]) (CRWMS M&O 2001 [153933])
Near Field Environment	(CRWMS M&O 2001 [153935])
Engineered Barrier System Degradation, Flow, and Transport	(CRWMS M&O 2001 [153001])
System-Level and Criticality	(CRWMS M&O 2000 [144180])

The FEP analysis and scenario development approach that was adopted for the TSPA-SR was based on the methodology developed by the NRC (Cranwell et al. 1990 [101234], Section 2). The approach is fundamentally the same as that used in many performance assessments, including the most recent analysis of the proposed repository by the NRC (Wescott et al. 1995 [100476], Chapter 3). The approach has also been used by the U.S. Department of Energy (DOE) for the Waste Isolation Pilot Plant (DOE 1996 [100975], Section 6.2), and by scientists working on repository programs in other countries (Bonano and Baca 1994 [105014]).

Subsequent to the completion of the FEP AMRs and the YMP FEP Database to support TSPA-SR, several internal and external FEP reviews were performed, as summarized in Section 3.1 of *Enhanced FEPs Plan* (BSC 2002 [158966]). The *Enhanced FEPs Plan* (BSC 2002 [158966]), was developed to address those FEP reviews, and to identify specific enhancements to the FEP analysis approach to support LA. These enhancements include a team approach for consistency (Section 3.2.1) and specific aspects of the FEP analysis (Section 3.2.2). The FEP AMRs will be updated as necessary for the TSPA-LA.

3.2.1 Interface Team for FEPs

A team approach will be used to provide for consistency in the identification and screening of FEPs for the TSPA-LA (see Section 3.2 of *Enhanced FEPS Plan* (BSC 2002 [158966])). FEP Team members will include a FEP Team Lead (FTL), and FEP experts, selected from within the Performance Assessment Strategy and Scope subproject group.

The FTL will manage the process of implementing the *Enhanced FEPs Plan* (BSC 2002 [158966]), with support from the FEP experts. A FEP AMR Lead and one or more SMEs will be identified for each of the subject areas listed in Table 3.2-1. The FEP AMR Leads are responsible for ensuring that relevant FEPs are treated appropriately within their FEP AMRs. The SMEs are the personnel most knowledgeable about individual FEPs and are responsible for developing explicit screening discussions for documentation in the FEP AMRs. The FEP AMR Leads and SMEs will be designated by various other subproducts within the Performance Assessment Project. The FEP Team will work closely with the FEP AMR Leads and SMEs.

3.2.2 FEP Analysis for TSPA-LA

For TSPA-LA, the FEP analysis and scenario development approach is the same as for TSPA-SR, but the five steps listed in Section 3.2 are described slightly differently so that they correspond more directly with the review methods and acceptance criteria in the *Yucca Mountain Review Plan* (CNWRA 2002 [158449], Section 4.2.1.2.1). The five steps for FEP analysis and scenario development for LA are illustrated in Figure 3.2-1 and are outlined below:

1. Identify and classify FEPs potentially relevant to the long-term performance of the disposal system.
2. Screen the FEPs using regulatory probability and consequence criteria to identify those FEPs that should be included in the TSPA analysis and those that can be excluded from the analysis.
3. Form scenario classes from the retained (included) FEPs, as appropriate.
4. Screen the scenario classes using the same criteria applied to the FEPs to identify any scenario classes that can be excluded from the TSPA.
5. Specify the implementation of the scenario classes in the computational modeling for the TSPA, and document the treatment of included FEPs.

FEP analysis and documentation, which includes Steps 1 and 2 above, is further described in this section. These steps address Scenario Analysis Acceptance Criteria 1 and 2, respectively, as outlined in the *Yucca Mountain Review Plan* (CNWRA 2002 [158449], Section 4.2.1.2.1.3). Scenario development, which includes Steps 3 and 4 above, is further described in Section 4. These steps address Scenario Analysis Acceptance Criteria 3 and 4, respectively, as outlined in the *Yucca Mountain Review Plan* (CNWRA 2002 [158449], Section 4.2.1.2.1.3). Implementation of the scenarios in TSPA models (Step 5 above) is described in Section 5.3.

The current status of FEP analysis is summarized below. Specific enhancements under consideration for TSPA-LA described in the *Enhanced FEPs Plan* (BSC 2002 [158966], Section 3.2) are also noted.

Step 1: Identification and Classification of FEPs–An initial list of FEPs relevant to Yucca Mountain was developed from a comprehensive list of FEPs from radioactive waste disposal programs in other countries (Freeze et al. 2001 [154365], Section 2.1) and was supplemented with additional YMP-specific FEPs from project literature, technical workshops, and reviews (Freeze et al. 2001 [154365], Sections 2.2 through 2.4). The YMP FEP list may be expanded if additional FEPs are identified during the LA process.

The all-inclusive FEP identification approach produced approximately 1,800 specific FEPs, and resulted in considerable redundancy in the FEPs list, because the same FEPs were frequently identified by multiple sources. To eliminate the redundancy and to create a more efficient aggregation of FEPs to carry forward into the screening process, each of the specific FEPs was classified according to a process and criteria described in Section 3.2 of the *FEP Database Report* (Freeze et al. 2001 [154365]). The classification process was designed to produce a subset (referred to as primary FEPs) of the approximately 1,800 initially identified FEPs that captured all of the issues relevant to the postclosure performance of the proposed repository. For TSPA-SR, the classification process resulted in 323 primary FEPs (CRWMS M&O 2000 [153246], Appendix B), each of which encompassed a single process or event, or a few closely related or coupled processes or events that could be addressed by a specific screening discussion.

Subsequent to TSPA-SR, an updated list of 328 primary FEPs was produced. This updated FEP list corresponds to REV 00 ICN 01 of the *FEP Database Report* (Freeze et al. 2001 [154365]). The origin of the additional FEPs and other changes from TSPA-SR are summarized in Section 5.5 of the *FEP Database Report* (Freeze et al. 2001 [154365]). These new FEPs were added to enhance traceability. They did not result in any changes to TSPA or process models.

The current version of the YMP FEP Database STN 10418.2-00 (BSC 2002 [159684]) contains the same 328 FEPs as REV 00 ICN 01, and the technical information consistent with the list of FEP AMRs in Table 3.2-1.

Enhancements to Step 1 for TSPA-LA include:

- Develop a hierarchical classification scheme that facilitates navigation within the database for reviewers and, where possible, parallels the structure used to describe TSPA-LA. This will improve transparency and traceability, but will not change the number or screening of FEPs.
- Refine the existing FEP list for consistency with the new classification scheme and for a more consistent level of detail between FEPs. This will not change the technical content of the overall FEP list, but may result in a minor change in the number of FEPs due to re-organization of certain FEPs.
- Provide an ongoing systematic process for configuration management, evaluation and tracking of potential new FEPs and changes to existing FEPs.

Step 2: Screening of FEPs–Each of the 328 FEPs is screened for inclusion or exclusion in the TSPA on the basis of probability or consequence criteria, developed from 10 CFR Part 63. The criteria are outlined below:

- **Probability (10 CFR 63.114(d)).** Consider only events that have at least one chance in 10,000 of occurring over 10,000 years. FEPs not meeting this criterion may be excluded (screened out) from the TSPA on the basis of low probability. For example, meteorite impact was excluded because of low probability.
- **Consequence (10 CFR 63.114(e) and (f)).** Specific FEPs must be evaluated in detail if the magnitude and time of radiological exposures or radionuclide releases would be

significantly changed by their omission. FEPs not meeting this criterion may be excluded (screened out) from the TSPA on the basis of low consequence. For example, erosion and sedimentation were excluded because of low consequence, even though they are certain to occur.

FEPs that are inconsistent with specific analysis requirements in 10 CFR Part 63 may also be excluded (screened out) from the TSPA. The most notable examples are FEPs that are inconsistent with regulatory specification of the human intrusion analysis and/or the characteristics of the receptor.

For certain FEPs, the 10 CFR Part 63 regulations provide guidance on whether the FEP is to be included or excluded. For example, for the reference biosphere, 10 CFR 63.305 states that the DOE should not project changes in society, the biosphere (other than climate), human biology, or increases or decreases of human knowledge or technology. Therefore, any FEPs related to these types of changes to the reference biosphere are excluded by regulation. Similar specifications exist for the characteristics of the reasonably maximally exposed individual (RMEI) (10 CFR 63.312) and for the human intrusion analysis (10 CFR 63.322).

The FEP screening process for TSPA-SR, illustrated in Figure 3.2-2, was performed by SMEs and documented in the FEP AMRs for the TSPA-SR (Table 3.2-1). The initial database began from an Organisation for Economic Co-operation and Development (OECD)-Nuclear Energy Agency (NEA) international database of generic FEPs potentially relevant to TSPA (Safety Assessment Management (SAM) 1997 [139333]). Specific guidelines for the basis of screening decisions and the content of screening documentation are outlined in the *FEP Database Report* (Freeze et al. 2001 [154365], Section 4.2). Of the 328 primary FEPs, 176 were included in the TSPA-SR analyses.

Enhancements to Step 2 under consideration for TSPA-LA include:

- Update screening discussions for consistency with final 10 CFR Part 63, where necessary.
- Enhance screening arguments to ensure adequate technical basis for excluded FEPs, where necessary (i.e., make specific reference to criteria in 10 CFR 63.114(d) through (f) and ensure that the technical bases for NRC expectations in the *Yucca Mountain Review Plan* (CNWRA 2002 [158449], Section 4.2.1.2.1.3) have been addressed).
- Enhance documentation for included FEPs, where necessary. This includes explicit references to included FEPs in technical AMRs and documentation of the mapping of included FEPs to TSPA model components.

General FEP Analysis Enhancements for TSPA-LA–Updates to the screening decisions are anticipated for a few FEPs based on post-TSPA-SR analyses including (1) *SSPA,* Volume 1 (BSC 2001 [155950]) and Volume 2 (BSC 2001 [154659]); (2) *Total System Performance Assessment—Analyses for Disposal of Commercial and DOE Waste Inventories at Yucca Mountain—Input to Final Environmental Impact Statement and Site Suitability Evaluation* (Williams 2001 [157307]), also referred to as the *TSPA FEIS Report*; and (3) *Total System*

Performance Assessment Sensitivity Analyses for Final Nuclear Regulatory Commission Regulations (Williams 2001 [156743]). Two examples are provided below:

- Seismic (vibratory ground motion) effects on rockfall and the associated effects of rockfall on drip shields and waste packages. These were excluded in TSPA-SR, but will be included as part of a new seismic scenario in TSPA-LA (see Section 4.3).
- Seismic (vibratory ground motion) direct shaking effects on drip shields, waste packages, cladding, and pallets. Only seismic vibration of cladding was included in TSPA-SR (as part of the nominal scenario class). Seismic vibration will be included as part of a new seismic scenario class in TSPA-LA (see Section 4.3).

Other enhancements identified in the *Enhanced FEPs Plan* (BSC 2002 [158966], Section 3.2), include:

- Updates to the FEP AMRs documenting new and changed FEPs and screening discussions. These will be delivered in support of TSPA-LA.
- Upgrades to the FEP Database to improve navigational capabilities and ensure consistency with the changes to the classification scheme and to the technical content of any of the FEPs. The final YMP FEP Database will be prepared to be consistent with the FEP AMRs that support TSPA-LA.
- Updates to the *FEP Database Report* (Freeze et al. 2001 [154365]) documenting changes to FEP analysis approach for LA. This will accompany the final YMP FEP Database in support of TSPA-LA.

3.3 MODEL FORM UNCERTAINTY: ALTERNATIVE CONCEPTUAL MODELS

Development of alternative conceptual models (ACMs) is a technique to specifically acknowledge model form uncertainty. In 10 CFR 63.114(c), the NRC specifically requires the DOE to "Consider alternative conceptual models of features and processes that are consistent with available data and current scientific understanding and evaluate the effects that alternative conceptual models have on the performance of the geologic repository." This consideration of ACMs is also incorporated into KTI 4.01, as noted in Appendix B (Meserve 2001 [156977]). The *Guidelines Document* (BSC 2002 [158794]) outlines a process for evaluating ACMs that is overseen by the ATL and discussed in Section 3.3.1. The *Guidelines Document* (BSC 2002 [158794]) introduces a process to consistently document the creation and screening of ACMs by various SMEs. This portion of the process is reviewed in Section 3.3.2. Those ACMs thought reasonable (based on, for example, precedent established by other analysts) and significantly different (based on, for example, differences in results) are passed on to TSPA analysts for their evaluation. This process is reviewed in Section 3.3.3. The impact of ACMs on TSPA-LA is reviewed in Section 3.3.4. The need to reevaluate FEP screening is mentioned in Section 3.3.5, and general aspects of the documentation are reviewed in Section 3.3.6.

3.3.1 Interface Team for ACMs

To provide consistency in addressing ACMs, the *Guidelines Document* (BSC 2002 [158794]) identifies two essential participants on the ACM interface team: the ATL and the SME. Various TSPA analysts and process modelers will provide technical support at the request of the ATL and SME. The term, "Abstraction Team Lead," is intentional because the person directing the consideration of alternative conceptual models can be the same individual that is used to address model abstraction issues. One ATL has been designated to address all ACMs from across the various subject areas to provide for consistency in the guidance given to the multiple SMEs on the appropriateness of proposed ACMs. The goal of establishing an ATL is to provide even-handedness in introducing ACMs. The ATL will be vigilant in selecting ACMs such that their use neither introduces specious ACMs nor neglects to introduce important ACMs in the TSPA-LA. The process provides for review and concurrence by the ATL and the SME prior to implementation of the alternative conceptual models in the TSPA-LA. It also specifies that the implementation of ACMs in the TSPA-LA be checked and reviewed by both the ATL and SME.

3.3.2 Identification and Screening of ACMs

The first activity in identifying and screening ACMs is to determine whether any ACMs are consistent with available data and scientific understanding. The consistency with available data and scientific understanding, and the reasonableness of ACMs, was previously considered and documented by the SMEs as part of the TSPA-SR process, although in varying degrees of detail (e.g., the various process model reports (PMRs) list several ACMs that were not incorporated to TSPA analyses, and external reviewers have identified ACMs not incorporated to TSPA analyses). This first activity requires the SMEs, in consultation with the ATL and TSPA analysts, to carefully examine the existing models; to identify previously considered ACMs; and to reevaluate their consistency with data in light of current project knowledge and supporting documentation used for the TSPA-SR, SSPA, and the TSPA-FEIS. For example, the consideration of stress corrosion cracking can be represented by more than one ACM. Since it was appropriate for the site recommendation, only the conservative model was chosen for use in *TSPA-SR* (CRWMS M&O 2000 [153246]). However, for TSPA-LA uncertainty in models will be considered and possibly analyzed, so the use of previously considered ACMs is being re-evaluated.

The SME will also review the model sensitivities/key parameters identified in the TSPA-SR, SSPA or other project documents (to be provided by the ATL) to identify where the use of ACMs would be most appropriate and suitable for implementation into TSPA-LA. That is, the SMEs should allocate their time to those ACMs that past experience has shown are an important influence on the results (according to a risk-informed approach). However, the intent is not to exclude ACMs that might show an impact simply because the original ACM did not show an impact. The SME will also reexamine FEPs to determine the appropriateness of modifying an existing screening decision (i.e., change from exclude to include) or identifying areas where an alternative treatment is appropriate.

The SME will determine if one or more conceptual models differ significantly from the existing conceptual model, are consistent with available data and current scientific understanding, and are reasonable. The definition of ACM in 10 CFR 63.114(c) includes the phrase "consistent with available data and current scientific understanding." Thus, a proposed model should be disqualified if it is verifiably inconsistent with any of the information. (Any model of a real system could eventually be shown not to agree with all the data in every instance since it is not the real system, but rather a model; hence, each ACM must be consistent with the available data in those areas that are important to the analysis.) The screening would first be done qualitatively, based on the technical judgment of the SME. If ACMs could not be screened out with a qualitative evaluation, then it would be necessary to develop the appropriate mathematical and computational models. However, the ACM may often be a variation of some base-case, in which case existing qualified computational software could be used.

The initial examination of ACMs will be documented in the corresponding model report. This documentation will include a list of the ACMs reviewed by the SME, the decision made regarding consistency with available data and scientific understanding and reasonableness, and the basis for the decisions made. If, in the judgement of the SME, only one conceptual model is consistent with all information, then uncertainty from associated ACMs is not significant. Additional uncertainty may be incorporated if more than one ACM is deemed appropriate for use, but they are not all passed individually to the TSPA model.

3.3.3 ACM Evaluation for Use in TSPA-LA

The responsible SME will evaluate whether any retained ACMs for the process being modeled should be developed further. For example, the SME may present results from process models to demonstrate that the ACMs do or do not produce significantly different results for the subsystem model. The ATL will review the SME recommendations. The ATL is responsible for determining which, if any, ACMs to implement in the TSPA-LA and for recommending the approach for implementation. If all ACMs predict behavior similar to the existing subsystem component used in the TSPA-FEIS, then ACM uncertainty is insignificant. In this case, the ATL will determine which one of the ACMs and existing subsystem components to carry forward to the TSPA-LA. The ATL will advise the SME of the determination, the determination will be documented in the model report by the SME, and a brief summary of this determination will be included in the TSPA-LA documentation by the ATL.

If differences in results from ACMs appear to be significant at the subsystem level, the next usual activity is for the SME (and process modelers) to develop appropriate model abstractions (see Section 3.4 for additional information on abstractions), based on the ACMs, for inclusion in the TSPA-LA. However, it is possible that building abstractions would not be necessary; conceivably, an underlying process model might not exist for the phenomena under consideration (e.g., curve fits to experimental data) and, consequently, abstractions would have been used directly in the evaluation at the subsystem level. The abstraction of phenomena into TSPA-LA is the same for each ACM and is discussed more completely in Section 3.4. Also, the OCRWM QA procedures require using validated models in the TSPA-LA, so eventually each abstraction of an ACM that is actually used in TSPA-LA would have to be validated (the definition of validation does not preclude having multiple valid ACMs; ACMs only used in preliminary analysis and later rejected and not used in producing results presented in TSPA-LA do not have to be validated). The major difference when multiple models are used to abstract phenomena is that differences between ACMs need to be evaluated at the total system level as discussed in the next section.

In some cases, the number of ACMs can be large. Although the general approach for modeling in TSPA-LA is to improve realism by reducing the number of conservative assumptions for parameter values, for ACMs the ATL and SME may still have to select what is perhaps the best ACM to use rather than quantitatively propagate multiple ACMs. Conservatism at the subsystem level (e.g., in the choice of a conservative ACM) will be used to define the best ACM to incorporate into TSPA-LA. In any case, the ATL and SME will provide a basis for that judgment, which will be documented in the relevant AMR.

3.3.4 ACM Impact Analysis in TSPA-LA

Should the total system level impact of any ACMs appear important enough to quantify for the TSPA-LA, one of two approaches will be used. For those ACMs for which little controversy exists (i.e., it is the SMEs judgment that any of the representations would be generally considered reasonable to the scientific community at large), TSPA analysts will incorporate the ACMs directly into the TSPA-LA. A parameter will be used to select between the two or more alternatives. This selection parameter will have a distribution assigned based on confidence as to the applicability of the various ACMs based on the SMEs judgment. Documentation of the technical basis for selection and weighting of ACMs will be included in the appropriate AMR.

The project plans to use weights to include multiple ACMs, in most cases; however, for especially controversial alternatives, the TSPA analyst may choose to run the full TSPA multiple realization simulation for each alternative and report the results. With this approach, it may be necessary to consider combinations of the ACMs. The project would first attempt to consider interactions (e.g., nonlinear coupling) of ACMs qualitatively, but if qualitative arguments are insufficient, the TSPA will also run various combinations of the ACMs to determine their significance to system performance.

3.3.5 FEPs

Guidance for the treatment of FEPs during consideration of ACMs is not different from guidance for FEPs in general. However, the SME must keep in mind that decisions concerning ACMs are not independent of decisions concerning FEPs. For example, if an ACM is already screened out by the FEP process, the SME should not include it. If the SME no longer believes it should be screened out, or if the ACM results in a different mechanism for including the FEP, the FEP should be further evaluated as a potential new FEP or a potential change to an existing FEP.

3.3.6 Documentation

A primary goal of the *Guidelines Document* (BSC 2002 [158794]) was to ensure that sufficient documentation was generated such that the NRC will understand all the uncertainty that contributes to how the mean dose is calculated in the TSPA, and whether the uncertainty comes from parameters or ACMs. Using the documentation, the NRC also should be able to assess whether the DOE has appropriately included ACMs.

For TSPA-SR, the description of the consideration and treatment of ACMs was placed in the appropriate AMRs. Similarly for TSPA-LA, all ACMs will be documented in the respective model reports in accordance with AP-SIII.10Q, *Models*. This documentation will likely be in the form of an attachment or distinct section to the model report, such that the updated documentation is more transparent than the existing documentation. The documentation for any ACM implemented into the TSPA-LA will include a qualitative description, unambiguous mathematical description of the model, and some form of validation. More detailed guidance on AMR documentation will be provided in an update to the *Scientific Processes Guidelines Manual* (BSC 2001 [157635]).

The TSPA-LA Model Document, prepared in accordance with administrative procedure AP-SIII.10Q, *Models*, will document how each ACM was implemented in the TSPA-LA. Additionally, an Appendix to the TSPA-LA Model Document will list each of the ACMs used or implemented in the TSPA-LA and provide a brief description.

3.4 MODEL FORM UNCERTAINTY: ABSTRACTIONS FOR USE IN TSPA-LA

As stated by the EPA in the preamble to 40 CFR Part 197 (66 FR 32074 [155216], p. 32102): "Simplifications and assumptions are involved in these modeling efforts out of necessity because of the complexity and time frames involved, and the choices made will determine the extent to which the modeling simulations realistically simulate the disposal system's performance. If choices are made that make the simulations very unrealistic, the confidence that can be placed on modeling results is very limited."

Often the term *abstraction* is applied to any simplification done to move from the real world, to a conceptual model, to a mathematical model, to a computational model, and then to the applied model. However, on the YMP, the term is used to distinguish between models that include details of the physical and chemical phenomena of a process under consideration (i.e., process models), and total system submodels (i.e., abstraction models) that are generally less complex than the process model but ideally capture the essence of the process model that is important to the total system model. The use of model abstractions can be a method to gain computational speed at the system level. The use of model abstractions is particularly appropriate when the abstraction does not pertain to a key or sensitive parameter or sensitive model component in a performance assessment. Several possible techniques or combination of techniques can be used to simplify the process model for use in the total system model as described in the *TSPA-SR* documentation (CRWMS M&O 2000 [153246], Appendix A, Section A.2). These include: (1) discretization of results from process models into lookup tables, (2) development of response surfaces (i.e., polynomial fits to results), (3) description of results as probability distributions, (4) development of linear transfer functions, and (5) reduction of dimensionality. Applicable standards will be utilized for submodel or abstraction development (e.g., ASTM C1174-97 [105725] will be used for waste package and waste form materials behavior submodels).

3.4.1 Interface Team for Abstraction

To provide consistency in implementation, documentation, and propagation of uncertainty and variability from the process model to the abstraction model, and in validation of the methods used in abstraction, the *Guidelines Document* (BSC 2002 [158794]) identifies two essential participants on the interface team for abstractions. As with the guidance on ACMs, these participants are the ATL and the SME. The guidelines indicate that one ATL will be designated to address all model abstraction issues across the various subject areas. The ATL will also serve as the team lead for addressing ACMs because of the interrelationship of these two subject areas.

3.4.2 Identify New and Revised Abstractions

The FEP screening process for TSPA-SR provides an initial basis for the models and model abstractions required in the TSPA-LA. It is expected that completely new abstractions will be rare. Rather, an important purpose of revised abstractions will be to characterize uncertainty better and remove conservatism. Hence, to support management of schedule risks described in Section 1.4, the need for new abstractions will consider their overall significance. With this strategy in mind, the ATL and TSPA analysts will meet to review the abstractions used in the TSPA-SR and TSPA-FEIS to identify any new or additional abstractions needed for the TSPA-LA. This identification will consider the findings of the TSPA-SR, SSPA, and previous sensitivity studies to identify the importance of various model components and consider the level of complexity or detail needed from the model abstraction by considering the level of resolution (simplification) of the other TSPA model components that the model abstraction feeds. Model abstractions that address key model components and/or key parameters will likely need a greater degree of detail than those that do not.

The ATL will initiate an interface meeting with the appropriate SMEs to discuss TSPA needs (e.g., a list of model components where additional model abstraction may be warranted) and learn of changes in model components proposed by the SMEs. The SME may identify technical issues in proceeding with a recommended model abstraction or may propose alternatives that would be more suitable for model abstraction. The SME will provide such information to the ATL for further consideration. For example, in some cases, the SME may advise that addressing parameter uncertainty and variability may be difficult if the current abstraction is used in which case new abstractions or a more detailed representational model may be required.

3.4.3 Develop Model Abstraction

In constructing the model abstraction, the SME (and process modelers) must consider the level of resolution of the process model and the level of resolution in the TSPA-LA model components. Consequently, the SME (and process modeler) will work in consultation with the ATL (and TSPA analysts) during the model abstraction development. This includes discussion regarding selection of any conservative components, parameter uncertainties, and evaluation of linear and nonlinear models when conservatism is used. The EPA notes in the preamble to 40 CFR Part 197 (66 FR 32074 [155216], p. 32102), "Inappropriate simplifications can mask the effects of processes that will in reality determine disposal system performance, if the uncertainties involved with these simplifications are not recognized." Consequently, the model abstractions used in the TSPA-LA must capture the important uncertainty and variability of the underlying process model. A description of how this uncertainty and variability was captured must be described in the corresponding model report. Often this uncertainty and variability will be captured through parameter distributions (Section 3.5); hence, the SME should also solicit input from the PTL to consider the feasibility of developing defensible parameter distributions.

The SME (and process modeler) are responsible for developing, validating, and documenting the model abstraction in the respective model report per the requirements of AP-SIII.10Q. The basis of the abstraction and the techniques used to develop the abstraction will be documented in such a way that they are clearly identifiable and explained to an external reviewer.

3.4.4 Incorporate Abstraction into TSPA-LA

To incorporate an abstraction into TSPA-LA, the TSPA analyst will obtain a controlled copy of any software and parameters needed to implement the model abstraction. Then, the TSPA analyst will integrate the model abstraction into the TSPA-LA model. The TSPA analyst will document the integration of the abstraction in the TSPA-LA Model Document. The ATL iterates with the TSPA analyst until the model abstraction is properly implemented and documented. If any changes are made to the abstraction for the purpose of integration, the TSPA analyst will ensure compliance with any applicable procedures. When the TSPA analyst's tasks are completed, the ATL and the SME perform a joint review of the integration activities, model report documentation, and abstraction results. The ATL also ensures that the development, description of the propagation of uncertainty and variability, and validation of the model abstraction are documented in the supporting model report.

3.4.5 Documentation

For TSPA-LA, the technical basis for an abstraction and the development and validation of the model abstraction will be documented in the corresponding model reports in accordance with AP-SIII.10Q, *Models*. As previously described for ACMs, this documentation will be provided as an attachment or distinct section to the model report such that the description is transparent. The documentation will include a qualitative description, an unambiguous mathematical description of the model abstraction, and validation of the model. Detailed guidance on the documentation will be provided in an update to the *Scientific Processes Guidelines Manual* (BSC 2001 [157635]).

As noted above, the TSPA-LA Model Document will document how the model abstraction was used in the TSPA-LA. The TSPA-LA Model Document will note any changes from the model abstraction (as documented in the respective model report), that were needed to integrate the model abstractions within the TSPA-LA. Applicable standards will be utilized for submodel or abstraction development (e.g., ASTM C1174-97 [105725] for waste package and waste form materials behavior submodels).

3.5 PARAMETER UNCERTAINTY: TSPA MODEL PARAMETERS AND DEVELOPMENT OF PARAMETER DISTRIBUTIONS

The NRC in 10 CFR 63.114(b) requires the DOE, in its TSPA, to "Account for uncertainties in parameter values and provide for the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment." The *Yucca Mountain Review Plan* (CNWRA 2002 [158449], Section 4.2) stipulates that the TSPA-LA model will be reviewed, in part, to identify whether the parameter ranges and distributions are technically defensible and whether they appropriately represent uncertainty. This review of parameter distributions will consider the relevant information and the corresponding uncertainty in the underlying information. In turn, the review will evaluate the effects of the parameter uncertainty on performance of the repository. This review will include an evaluation of the potential for inappropriate characterization of risk ("risk dilution") (i.e., the lowering of the risk, or dose, from an unsupported parameter range and distribution).

Internal and external reviews of YMP documents developed for the site recommendation, including the *TSPA-SR* (CRWMS M&O 2000 [153246]), found inconsistencies in the processes and methods used to develop and document all types of uncertainties, including parameter uncertainty. These reviews are summarized and evaluated in *Uncertainty Analyses and Strategy Letter Report* (Williams 2001 [157389]). In addition, this document (Williams 2001 [157389]) identifies strategies to meet the 10 CFR 63.114(b) requirement cited above in the TSPA-LA. A key component of these strategies was to develop guidance on the treatment of parameters and parameter uncertainty. This guidance is documented in Section 4 of the *Guidelines Document* (BSC 2002 [158794]) and summarized here. The guidance will be implemented in the TSPA-LA to provide for consistent treatment in categorizing, quantifying, evaluating, and documenting parameters and parameter uncertainties. As mentioned at the end of Section 3.1.1, the parameter uncertainty here will focus on epistemic uncertainty, as the aleatory uncertainty will be addressed as applicable in the supporting process and abstraction models.

3.5.1 Parameter Development Team

The process of characterizing parameter uncertainty must be tailored to the amount and type of information available to support the parameter development and the use of the parameter in the TSPA models. Hence, a team approach will be used to provide for consistency in the identification and development of parameter uncertainty in TSPA-LA (see *Guidelines Document* (BSC 2002 [158794], Sections 1.3.1 and 4.2)). Key Parameter Development Team members will include the Parameter Team Lead (PTL) and SMEs. The PTL will manage the process of implementing the guidelines and will work closely with the SMEs to identify parameters and assure the uncertainty in the parameter is appropriately quantified for the TSPA-LA. The PTL will be assisted in this process by one or more experts in statistical analysis and uncertainty analysis.

The SMEs are generally the principal scientists that are most knowledgeable about individual process models and their uncertain input parameters. The SMEs will provide the technical expertise to identify, implement, and document the treatment of parameter uncertainty using the processes identified in the *Guidelines Document* (BSC 2002 [158794]). The PTL and SMEs will be supported by process modeler(s), TSPA analyst(s), and the TSPA-LA Input Database Administrator. The process modeler will assist the SME in the development, and documentation of appropriate parameters. The TSPA analyst will integrate the parameters into the TSPA-LA. The TSPA Data Base Administrator will work with the PTL to document the parameters in a controlled database that is directly linked to the TSPA GoldSim model. The functional roles for the different team members are as follows:

- Parameter Team Lead (PTL)–Individual assigned responsibility to lead the process for ensuring the consistent treatment and documentation of parameter values, parameter distributions, and parameter uncertainty used in the TSPA-LA model. The PTL will have access to experts in statistical analysis and uncertainty analysis to add their expertise to the process.
- Subject Matter Expert (SME)–Personnel who are most knowledgeable about individual process models and uncertain parameters associated with the process models. The SME is responsible for identifying and developing parameters (including values, distributions, and uncertainty) consistent with the *Guidelines Document* (BSC 2002 [158794]) for use in the TSPA-LA.
- Process Modeler–Personnel assigned to assist the SME in developing and implementing process models for use in the TSPA-LA model.
- TSPA Analyst–Personnel assigned to integrate parameters, ACMs and model abstractions in the TSPA-LA model.
- TSPA Database Administrator–Personnel assigned to set up and administer the parameter database, operate the software used to maintain the parameter database, enter parameter values and verify parameter value entry (approved by the PTL) into the parameter database.

These functional roles may or may not correspond directly with the existing or future PA Project organizational structure. However, it is expected that individuals selected for the PTL role and experts in statistical analysis and uncertainty analysis will be designated by, and report to, the TSPA Department and PA Strategy and Scope subproject managers. The SMEs will be designated by, and report to, the various PA Project departments and the respective subproject managers. This allows for the input and documentation to the TSPA-LA model to be controlled within the PA Project.

3.5.2 Identify TSPA Model Parameters

To initiate the process of identifying TSPA model parameters and for any newly developed models for TSPA-LA, the PTL and TSPA analysts will describe the computational model (implemented mathematical model) in the TSPA and identify the set of TSPA model simulation settings and model input parameters that are necessary to perform the calculations.

TSPA model simulation settings will be officially tracked when a TSPA-LA model simulation is warehoused in Technical Data Management Systems (TDMS). Model input parameters will be categorized by the PTL as fixed (e.g., single value) or uncertain. Example input parameters are listed in Appendix F.

The TSPA for Yucca Mountain has historically included a large number of parameters defined by probability distributions (approximately 300) (see Table F-1 for examples of such parameters that are identified as uncertain). Though the uncertainty in most of these parameters is not important to explain the variation in the overall dose calculation, the approach of including a large number of parameters with uncertain values will be continued to ensure that TSPA-LA is able to identify parameters that might become more important because of changes in the system models or because of changes in the values or distributions for parameters.

3.5.3 Develop Fixed Parameter Values

In those few instances when a model-configuration parameter is fixed at a single value in TSPA-LA, either the mean of the distribution (as developed below) will be used, or a recognized "best estimate" as defined by the Parameter Development Team will be used.

3.5.4 Develop Distributions for Parameter Uncertainty

The TSPA analyst will describe the pertinent TSPA model component and pertinent parameters to the SME and PTL. In turn, the SME describes the pertinent information for developing model parameters and their uncertainty to the TSPA analyst and PTL. The SME is responsible to evaluate all relevant sources of information in order to fully characterize the uncertainty in the parameter value. The source of underlying information will be documented on a Parameter Entry Form (example shown in Figure 3.5-1) or equivalent memorandum.

The Parameter Development Team (PTL, SME, and TSPA analyst) will develop a parameter distribution for uncertain parameters as follows.

Step 1–SME evaluates the sources of information available to support the development of the parameter in question. These sources may consist of either direct observations (based on testing or other analyses) or more quantitative analyses including the output of process or abstraction models. Because the approach for quantifying TSPA input parameter uncertainty may depend on the type of parameter considered, two determination paths, Step 2 or Steps 3 and 4 are presented.

Step 2–In many cases sufficient information exists for the PTL, working with the SME and TSPA analyst, to directly develop the parameter used as input to the TSPA-LA model as well as the uncertainty in that parameter. Examples of this include radionuclide solubilities, sorption coefficients, corrosion rates, etc. In these instances, the parameter uncertainty used as input to the TSPA model can be directly evaluated based on the observations, considering the spatial and temporal representations of the observations. As an example, the team might construct an empirical piecewise-linear cumulative distribution function. Other distributions such as the normal or gamma may be developed using the method of maximum likelihood or moments and test for their goodness-of-fit using a chi-square or Kolmogorov-Smirnov statistical test. Alternatively, the team might assume each observation is an estimate of the mean and then, assuming a Bayesian viewpoint, fit a Student-t or normal distribution using the method of moments such that the uncertainty in the true mean could be described. If a distribution is developed at this step, proceed to Step 5.

Step 3–In cases where the TSPA input parameter is based on the output (i.e., abstraction) from analyses using detailed process models, the approach to quantify parameter uncertainty depends on the type and structure of the underlying process model. Besides developing functional abstractions as alluded to in Section 3.3 and 3.4, some process models can be run for multiple realizations and the result abstracted as a parameter distribution. An example of this in the TSPA-SR is the biosphere dose conversion factors. Other, more complicated process models will only be run for a sufficient number of discrete cases to adequately capture the range of outcomes. Examples of this include the drift-scale thermal-hydro-chemical model, and the unsaturated zone flow model. When distributions must be supplied for the parameters of the functional abstractions alluded to in Sections 3.2 and 3.4, the PTL requests that the SME provide estimates that subjectively account for the range of possible outputs. This range must consider other sources of uncertainty in the input to the model. Specifically, these subjective estimates include:

1. The range of the parameter (i.e., the minimum and maximum values taken by the parameter), if possible, and
2. One of the following (in decreasing order of preference):
    a. Percentile points for the distribution of the parameter (e.g., the 25^{th}, 50^{th} [median], and 75^{th} percentiles),
    b. Mean value and standard deviation of the distribution, or
    c. Mean value.

The range and distribution for the parameter must take into account the model form and the treatment of input uncertainty in the TSPA analysis (see Section 4.1.2 of the *Guidelines Document* (BSC 2002 [158794])). For example, if the abstracted component of the TSPA model does not discretize spatially or temporally, then the parameter distribution must account for this temporal or spatial variability (aleatory uncertainty) in a suitably averaged manner. The PTL is responsible for assuring consistency in the application of the methods and the appropriateness of the estimates. To set a range too narrowly or broadly could bias the mean and violate the intent of 10 CFR 63.304(4):

> "…Characteristics of reasonable expectation include that it: …(4) Focuses performance assessments and analyses on the full range of defensible and reasonable parameter distributions rather than only upon extreme physical situations and parameter values…"

Step 4–The PTL, in consultation with the SME and TSPA analyst, will construct a distribution depending upon the kind of subjective information that has been provided in Step 3. The construction will be in accordance with published results from informational entropy theory to the extent practicable (see Section 4.1.2 of the *Guidelines Document* (BSC 2002 [158794])). The Project anticipates that only a small subset of the many types of distributions possible will be necessary. Examples of the type of distribution suggested from the application of maximum entropy include the following as explained by Harr (1987 [100580]) and Tierney (1990 [125989]):

1. Uniform probability distribution function (PDF) based on the subjective range of the parameter provided in Step 3,
2. Piecewise-linear cumulative distribution function (CDF) based on the range and subjective percentiles provided in Step 3,
3. Exponential PDF (truncated) based on the subjective range and mean value,
4. Normal PDF based on the subjective mean value and standard deviation,
5. Normal PDF (truncated) based on the subjective range, mean value and standard deviation.

Step 5–The SME and TSPA analyst of the Parameter Development Team will review the distribution suggested by the PTL and, as appropriate, revise the distribution to fully evaluate the uncertainty. The Project will rely upon the expertise residing in the Parameter Development Team to apply any specific methods appropriate to incorporate any other information pertinent to the parameter. Concurrence by all three members of the team is signified by signatures on a Parameter Entry Form (example in Figure 3.5-1) or equivalent memorandum. Normally, the PTL mediates informal disputes in assigning a distribution. If the PTL cannot resolve a dispute, the TSPA Department Manager will facilitate informal dispute resolution. If the dispute must be resolved formally, the dispute over the Parameter Entry Form may be resolved, using the procedure for *Resolution of Differing Professional Opinion* (AP-ENG-004 [159727]).

After completing the parameter development as documented on the Parameter Entry Form (see Figure 3.5-1) or equivalent memorandum, the SME will include this form or memorandum as part of the Analysis or Model Report, as previously mentioned. In addition, the SME will submit the form or memorandum and an attachment that describes the sources of information ("roadmap") as part of the DTN submittal to the Technical Data Management System (TDMS) to provide sufficient information to understand the DTN so that another user (specifically, personnel supporting the TSPA inputs database) can easily access that individual parameter.

Finally, to facilitate populating the TSPA-LA inputs database, the SME will also provide a copy of the completed Parameter Entry Form to alert the TSPA-LA Database Administrator that a parameter assignment has been completed and stored in TDMS. The TSPA-LA Database Administrator will then assign personnel supporting the TSPA-LA Inputs Database to obtain (from TDMS) the endorsed values and distribution for the parameter using the appropriate DTN along with the Parameter Entry Form and attached roadmap. If the road-map instructions do not allow the parameter to be identified and accessed in a reasonable period of time, the TSPA-LA Database Administrator will notify the PTL that this problem exists. The PTL will then work with the SME to revise the road-map information so that the parameter can be efficiently identified and accessed.

Ideally, the parameter set used in the TSPA-LA will be judiciously chosen by the SMEs developing the various abstractions to be statistically independent. Thus, the correlation between parameters will be minimal. For example, although the SME could use either (1) an average thermal conductivity and volumetric capacity parameter, or (2) solid thermal conductivity, matrix porosity, and lithophysal porosity parameters, the latter parameter set would be better since the correlation between parameters would be less. However, this simple choice is not always possible. In any case, the SME will be responsible for describing any correlations between parameters.

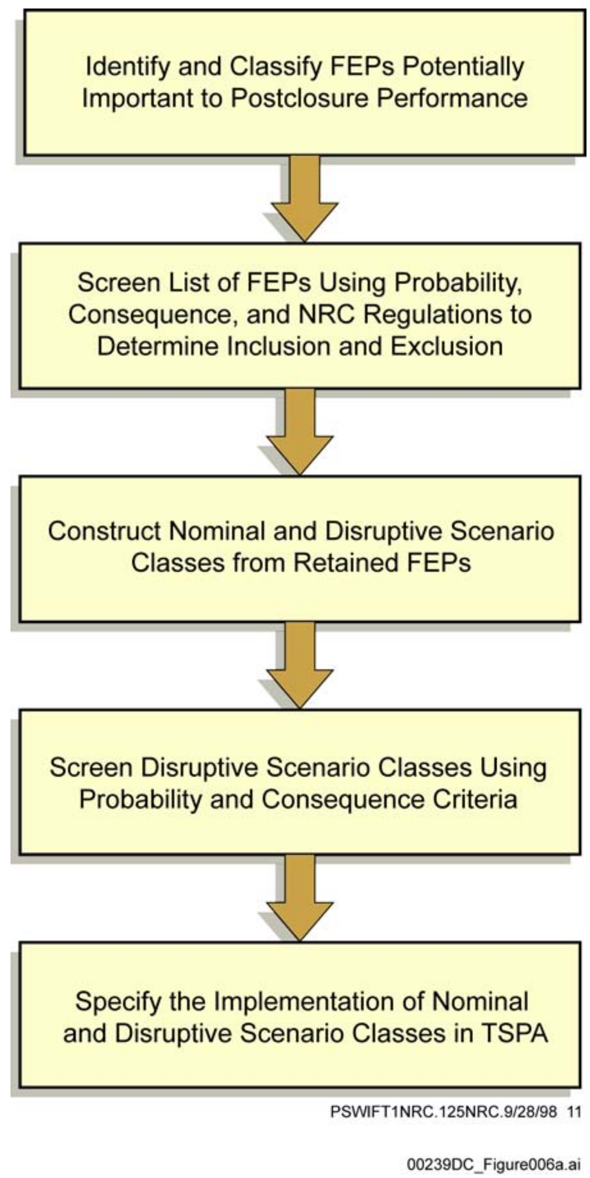
As the Parameter Development Team reviews and develops parameter distributions, they will focus attention on the reasonableness of the assumptions. They will be particularly watchful that the parameter distributions are not overly conservative or overly optimistic. The emphasis here is on representativeness of the uncertainty based on available information. By stressing reasonableness in the parameter distribution definitions, the likelihood of causing risk dilution (i.e., the underestimation of risk, or dose, due to the choice of insufficiently supported optimistic inputs) to the TSPA-LA should be reduced. A proactive approach to producing reasonable parameter distributions for input to the TSPA-LA analysis should reduce the potential for risk dilution. The most likely parameter distributions to cause risk dilution are those based in part on subjective inputs as the basis for their specification. These parameters will be identified by the Parameter Development Team for further inspection, including the examination of the TSPA-LA results for risk dilution.

The steps described in this subsection are intended to control the development of parameters and the associated uncertainty. Because the appropriate personnel are integrating regularly to determine the required parameter information, it is anticipated that the specified steps will be accomplished in a single meeting between the appropriate personnel as experience is gained, without too large of a burden of iterations and documentation between the personnel.

3.5.5 Documentation of TSPA Parameters

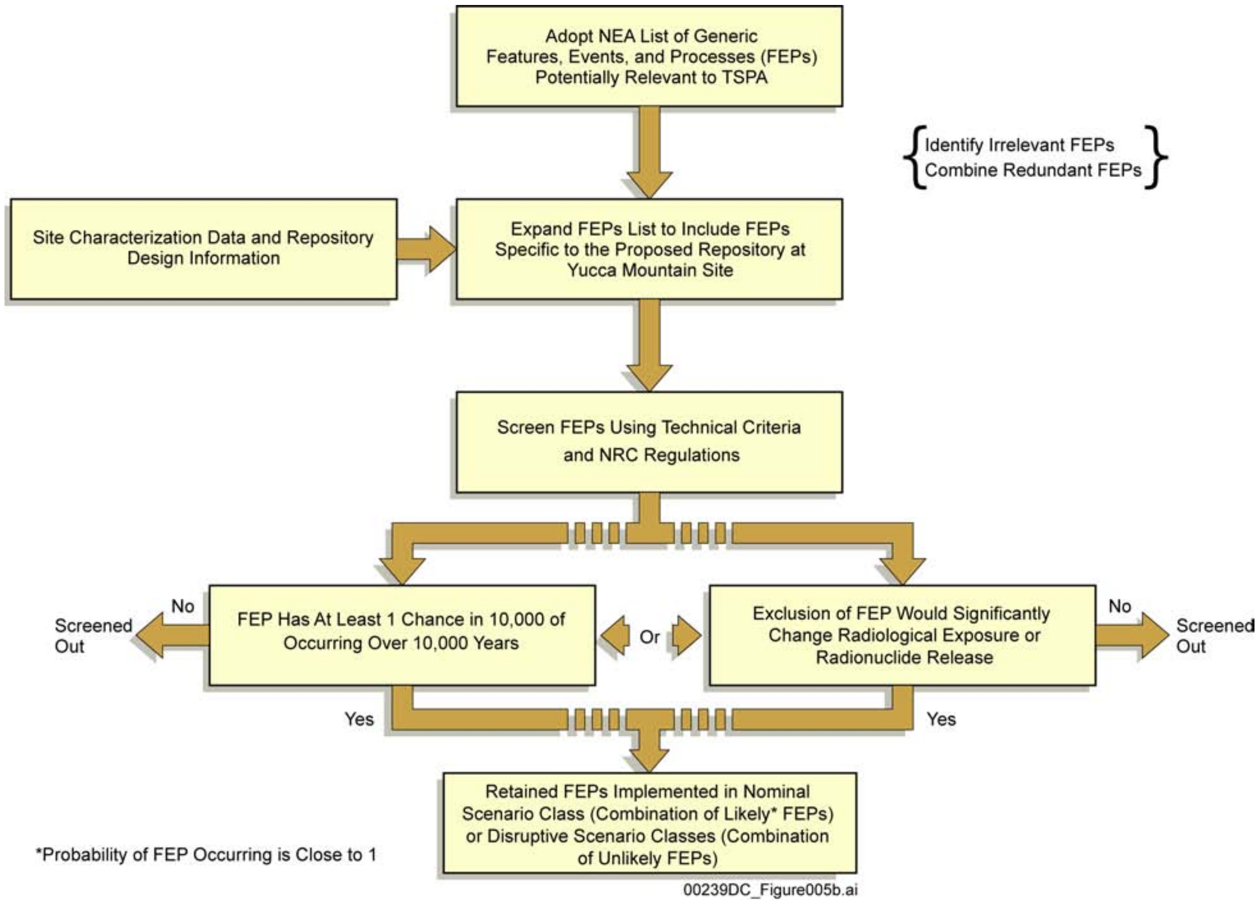
All TSPA-LA model parameters (both uncertain and certain) will be developed using the process described in Sections 3.5.3 and 3.5.4 and will be documented in the appropriate individual model or analysis report (AMR) by the SME according to AP-SIII.10Q*, Models* or AP-SIII.9Q *Scientific Analyses*. Each individual AMR will include an identification of process model parameters (Section 4 of the AMR), a detailed discussion of the uncertainties associated with the AMR inputs (Section 6 of the AMR), and a detailed discussion of all outputs developed in the AMR (Section 8 of the AMR). The discussion of AMR inputs and outputs will address the *Yucca Mountain Review Plan* acceptance criteria (CNWRA 2002 [158449], Section 4.2) that requires providing the technical bases for parameter values, assumed ranges, probability distributions, and bounding assumptions used in conceptual models, process models, and alternative conceptual models, considered in the TSPA-LA. More detailed guidance on AMR documentation will be provided in an update to the *Scientific Processes Guidelines Manual* (BSC 2001 [157635]). The PTL will work with SMEs revising AMRs for LA to implement the process outlined in Sections 3.5.3 and 3.5.4 for documenting model/analyses input and output parameters.

The output parameters (technical product output) from process model AMRs provide the inputs for the TSPA-LA model. Like the process model AMRs, the TSPA-LA Model Document will be prepared in accordance with AP-SIII.10Q, *Models*. The TSPA-LA Model Document (see Appendix C for a draft outline) will include an identification of TSPA-LA model input data and parameters in Section 4, a brief discussion of the uncertainties associated with the TSPA-LA model inputs (with references to supporting documentation for detailed discussion of the uncertainty in a particular parameter) in Section 6, and a detailed discussion of outputs developed in the TSPA-LA model in Section 8. The discussion of TSPA-LA Model Document inputs and outputs will address the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria that requires providing the technical bases for parameter values, assumed ranges, probability distributions, and bounding assumptions used in conceptual models, process models, and alternative conceptual models incorporated into the TSPA-LA.



Source: Modification of DOE 2002 [155943], Figure 4-156

Figure 3.2-1. Steps in the FEP Analysis and Scenario Selection Process



Source: DOE 2002 [155943], Figure 4-157

Figure 3.2-2. Schematic Illustration of the FEP Screening Process

<table>
<tr><td rowspan="2">YMP</td><td>Parameter Entry Form
Form Number: TBD</td><td>QA: ___
Effective: TBD</td></tr>
<tr><td colspan="2">Procedure: __N/A____ Revision: _________ Page _1__ of ___</td></tr>
</table>

☐ Modification	☐ Error Correction	☐ New	☐ Deactivation
Parameter:	____________	Id:	____________
Material:	____________	Idmtrl:	____________
Model:	____________	Idpram:	____________
Category:	____________	Units:	____________
Distribution:			
Type:		Mean:	____________
		Median:	____________
		Std Dev:	____________
Values:		Attachment:	Y N
Source: Interpretation:		Attachment:	Y N

Parameter Entry Approved By:

______________________ Parameter Team Lead (Print)　　______________________ Parameter Team Lead Signature/Date

Concurrence:

______________________ Subject Matter Expert (Print)　　______________________ Subject Matter Expert Signature/Date

______________________ TSPA Analyst (Print)　　______________________ TSPA Analyst Signature/Date

Entered By: ______________ *(Print)*　　______________ *Signature*　　__________ Date

Entry Checked by: ______________ *(Print)*　　______________ *Signature*　　__________ Date

Data Control　　PA Database ~　　Other ____________________ (i.e., input file)　　TDMS File Code: __________

Source: *Guidelines Document* (BSC 2002 [158794])

Figure 3.5-1. Example Parameter Entry Form

4. SCENARIO CLASSES FOR LA

A scenario is a well-defined, connected sequence of FEPs that describes a possible future condition of the proposed repository system. A scenario class is a set of related scenarios that share sufficient similarities that they can usefully be aggregated for the purposes of screening or analysis. The objective of scenario development is to define a limited set of scenario classes and scenarios that can reasonably be analyzed quantitatively while still maintaining comprehensive coverage of the range of possible future states of the disposal system. There are an essentially infinite number of possible future states, and for scenario development to be useful, it must generate scenario classes that are representative of the range of futures that are potentially relevant to the licensing of the facility.

The number and breadth of scenario classes depends on the resolution at which scenarios have been defined. Coarsely defined scenarios result in fewer, broad scenario classes, whereas narrowly defined scenarios result in many narrow scenario classes. In turn, the number and breadth of scenarios depends on the resolution at which FEPs have been defined. There is no uniquely correct level of detail at which to define scenario classes, scenarios, and FEPs. Decisions regarding the appropriate level of resolution for the analysis are made based on consideration of the importance of the scenarios, their effects on overall performance, and the resolution desired in the results. For efficiency, scenario classes, scenarios, and FEPs should be aggregated at the coarsest level at which a technically sound argument can be made, while still maintaining adequate detail for the purposes of the analysis.

As described in Section 3.2.2, FEP analysis and scenario development for TSPA-LA will follow the same process that was used for TSPA-SR. FEP analysis includes Steps 1 and 2 of this process, which were summarized in Section 3.2.2. Scenario development includes Steps 3 and 4 of this process. The status of these scenario development steps to support TSPA-LA is summarized below. These steps directly address Scenario Analysis Acceptance Criteria 3 and 4, respectively, as outlined in the *Yucca Mountain Review Plan* (CNWRA 2002 [158449], Section 4.2.1.2.1.3). These steps also indirectly address Event Probability Acceptance Criteria 1 through 5 from the *Yucca Mountain Review Plan* (CNWRA 2002 [158449], Section 4.2.1.2.2.3).

Step 3: Formation of Scenario Classes–All FEPs retained during the formal identification and screening steps (Steps 1 and 2, summarized in Section 3.2.2) are used for TSPA scenario class development.

The nominal scenario class is developed using all screened in FEPs that are expected to occur after closure (i.e., FEPs that have a probability of occurrence near 1.0, but that may have uncertain consequences). The nominal scenario class represents the most plausible evolution of the repository system and includes both favorable future conditions and potentially adverse future conditions. The disruptive event scenario classes are developed using combinations of screened in FEPs that have a low probability of occurrence (but greater than the screening probability criterion of one occurrence in 10,000 in 10,000 years) but may produce potentially adverse future conditions (i.e., radiological exposures or radionuclide releases would be significantly changed by their omission). Disruptive event FEPs are typically, but not necessarily, unlikely FEPs, which are defined in 10 CFR 63.342 to have a probability of occurrence of less than one chance in 10 and at least one chance in 10,000 of occurring in

10,000 years. Disruptive event scenario classes typically also include the nominal FEPs and represent low-probability perturbations to the expected evolution of the repository system.

For TSPA-SR, the disruptive event scenario class consisted of two igneous modeling cases: igneous intrusion and volcanic eruption (CRWMS M&O 2000 [153246], Section 2.1.2). Because only igneous modeling cases were included, it was also referred to as the igneous scenario class. As noted in Section 3.2.2, the expected inclusion of additional seismic FEPs (i.e., the effects of extreme vibratory ground motion due to unlikely seismic events on rockfall, drip shields and waste packages) for TSPA-LA will result in a seismic scenario class as one of the disruptive event scenario classes.

Human intrusion is a special case of a disruptive scenario class that is defined by regulation (10 CFR 63.321 and 10 CFR 63.322). Because of the regulatory guidance, the human intrusion case will be referred to as a stylized analysis for TSPA-LA rather than a scenario class. The approach to evaluation of this stylized case is described in Section 4.4.

Step 4: Screening of Scenario Classes–Scenario screening is used to identify scenario classes that contain a combination of FEPs whose combined probability of occurrence (or consequence) is low enough to permit exclusion from the TSPA, even though the probability (or consequence) of the individual FEPs requires them to be included. For a scenario class to be screened out, the combined low probability (or consequence) should not result from an inappropriately narrow scenario definition that artificially reduces the probability (or consequence) below the regulatory cutoff (CNWRA 2002 [158449], p. 4.2-9).

For TSPA-SR, detailed screening was performed on FEPs (as described in Section 3.2.2, Step 2). The scenario classes formed in Step 3 above were composed of those screened in FEPs. No additional exclusions were made during scenario screening. For TSPA-LA, additional screening is anticipated for the disruptive event scenario classes. The Latin Square method (NRC 2000 [153033], Section 3.2.5) is used to illustrate the combined probabilities of occurrence or non-occurrence of the igneous scenario class (I and I^-) and the seismic scenario class (S and S^-) (Table 4-1). The probabilities (P) of occurrence and non-occurrence for each scenario class sum to one. The probabilities of occurrence (I and S) are both expected to be quite low, such that the probabilities of non-occurrence (I^- and S^-) are near 1 (i.e., greater than 0.99).

Table 4-1 shows that the combined occurrence of the seismic and igneous scenario classes is expected to be screened out based on low probability. This probability-based screening relies on the independence of the seismic and igneous scenario classes. Although some seismicity is associated with igneous activity, the extreme seismic events considered in the seismic scenario class are expected to be shown to have tectonic rather than magmatic origins, and therefore be independent from igneous activity. However, a final screening decision for the combined occurrence of a seismic event (that produces significant drift collapse) preceding an igneous event will not be made until the associated probabilities and consequences have been fully evaluated. Table 4-1 also indicates the probability of the nominal scenario class, which is represented by the combined non-occurrence of the two disruptive scenario classes.

Table 4-1. Latin Square Diagram for an Analysis with Two Disruptive Scenario Classes

	Seismic Occurs, S [P = P(S)]	**Seismic Does Not Occur, S^-** [P = 1 – P(S) ≅ 1]
Igneous Occurs, I [P = P(I)]	**I S** [P < 10^{-4} in 10,000 yrs] **Expected to be Screened Out**	**I S^-** [P ≅ P(I)] **Igneous Scenario Class**
Igneous Does Not Occur, I^- [P = 1 – P(I) ≅ 1]	**I^- S** [P ≅ P(S)] **Seismic Scenario Class**	**I^- S^-** [P = 1 – P(I) – P(S)] **Nominal Scenario Class**

Each of the TSPA-LA analysis cases (Nominal Scenario Class, Igneous Scenario Class, Seismic Scenario Class, and Human Intrusion Stylized Analysis) are described in more detail in Sections 4.1, 4.2, 4.3, and 4.4, respectively.

4.1 NOMINAL SCENARIO CLASS

The nominal scenario class contains a single modeling case that is composed of the set of expected FEPs, as determined by a formal FEP screening procedure described in Section 3.2.2. The TSPA-SR FEP screening basis and decisions are summarized in Appendix B of *TSPA-SR* (CRWMS M&O 2000 [153246]), but will be updated in the FEP AMRs (Table 3.2-1) to support TSPA-LA. The nominal scenario class for TSPA incorporates the important effects and system perturbations caused by climate change and repository heating that are projected to occur over the 10,000-year compliance period (Figure 4.1-1).

The nominal scenario class includes the following general processes:

- Unsaturated zone flow
- Engineered barrier system environment (including near-field thermal, physical, and chemical environments)
- Waste package and drip shield degradation
- Waste form degradation
- Engineered barrier system flow and transport
- Unsaturated zone transport
- Saturated zone flow and transport
- Biosphere

The technical basis for the conceptualization of the TSPA-SR nominal scenario class is summarized in *TSPA-SR* (CRWMS M&O 2000 [153246], Sections 3.2 through 3.9) and the *Yucca Mountain Science and Engineering Report* (DOE 2002 [155943], Section 4.2).

For TSPA-LA, the nominal scenario class is expected to include certain enhancements based on post-TSPA-SR analyses using the supplemental TSPA model (BSC 2001 [155950]; BSC 2001 [154659]) and the revisions for the final regulations (Williams 2001 [157307]; Williams 2001 [156743]). These enhancements for the TSPA-LA nominal scenario class are summarized in Table 5.1-1. Additional discussion of the implementation of the nominal scenario class in TSPA-LA is provided in Section 5.3.1.

4.2 IGNEOUS SCENARIO CLASS

The igneous scenario class (Figure 4.2-1) includes two distinct modeling cases: (1) volcanic eruption at the repository location and (2) igneous intrusion (or magmatic flooding) of some of the emplacement drifts in the repository. The technical basis for the conceptualization of the TSPA-SR igneous modeling cases are summarized in *TSPA-SR* (CRWMS M&O 2000 [153246], Section 3.10) and the *Science and Engineering Report* (DOE 2002 [155943], Section 4.3.2.1).

Both modeling cases assume that the eruptive event consists of a magmatic penetration of the repository facility after permanent closure. The conceptualization of the volcanic eruption modeling case assumes that the magma flow intersects and destroys waste packages, bringing waste to the surface through one or more eruptive conduits. For TSPA-SR, the atmospheric transport model (ASHPLUME) of radionuclides bound in the particles of volcanic ash, dispersed the particles downwind and ultimately deposited them on the ground at the RMEI location.

The igneous intrusion modeling case assumes that a hypothetical igneous dike intersects drifts of the repository and that the associated waste packages are damaged, exposing the waste within to percolating water. For TSPA-SR, models accounted for the additional waste package failures and analyzed the transport of radionuclides through the groundwater pathway to the location of the RMEI.

For TSPA-LA, the igneous modeling cases are expected to include certain enhancements based on post-TSPA-SR analyses using the supplemental TSPA model (BSC 2001 [155950]; BSC 2001 [154659]) and the revisions for the final regulations (Williams 2001 [157307]; Williams 2001 [156743]). These enhancements for the TSPA-LA igneous modeling cases are summarized in Table 5.1-1. Additional details of the implementation of the igneous modeling cases in TSPA-LA is provided in Section 5.3.2.

The probability of the igneous intrusion modeling case is equal to the probability of an intrusive event (i.e., a swarm of one or more dikes intersecting the repository). This is also referred to as the event probability. The probability of the volcanic eruption modeling case is equal to the intrusive event probability times the conditional probability of a conduit or vent forming within a drift (also referred to as the vent or conduit probability).

4.3 SEISMIC SCENARIO CLASS

Potential seismic effects on the underground facilities and waste packages were screened out of TSPA-SR (except for damage to cladding from vibratory ground motion). However, based on revised screening decisions (see Section 3.2.2), a seismic scenario class is expected to be included in TSPA-LA. The seismic scenario class will be based on a seismic probabilistic risk assessment. The general methodology is described in a letter report to the NRC (Brocoum, 2001 [159576]). Details of the implementation are described in Section 5.3.2. The seismic scenario class is expected to be composed of a single modeling case that includes the following processes (Figure 4.3-1):

- Effects of extreme vibratory ground motion on rockfall
- Effects of ground-motion-induced rockfall on drip shields, and on waste packages if a drip shield fails as a structural barrier
- Effects of direct ground-motion-induced shaking on drip shields, waste packages, cladding, and pallets.

Note that for TSPA-SR, seismic vibration of cladding was included as part of the nominal scenario class, but for TSPA-LA it will be included in the seismic scenario class. Direct effects of fault displacement, changes in fractures, faults, or hydrologic response are expected to be excluded from TSPA-LA based on current analyses.

The probability of the seismic scenario class is equal to the mean frequency of exceedance of extreme vibratory ground motion at the repository, which is based on the ground motion hazard curve from the *Probabilistic Seismic Hazard Analyses for Fault Displacement and Vibratory Ground Motion at Yucca Mountain, Nevada* (CRWMS M&O 1998 [103731]). The implementation of the seismic scenario class in TSPA-LA is expected to take the form of response surfaces that relate the level of ground motion to drip shield and waste package failed area as a function of wall thickness. The effective failed areas will include the combined effects of both rockfall and shaking. Additional details of the implementation of the seismic scenario class in TSPA-LA is provided in Section 5.3.2.

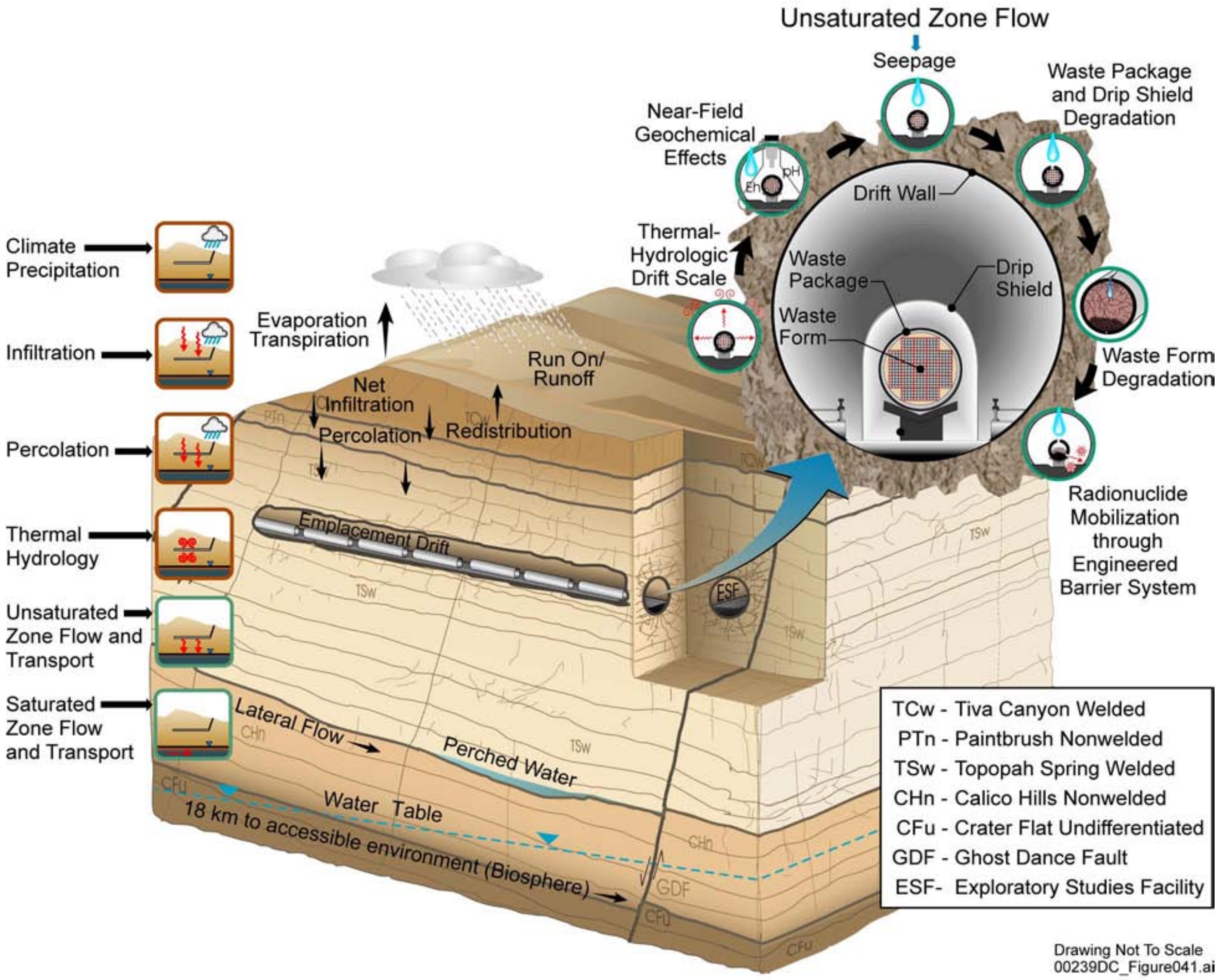
4.4 HUMAN INTRUSION STYLIZED ANALYSIS

The NRC regulation establishing the human intrusion standard, 10 CFR 63.321, requires compliance in licensing with the 15-mrem dose limit for individual protection if the DOE determines that, within the 10,000-year regulatory compliance period, the waste packages would degrade sufficiently that a human intrusion could occur without recognition by the driller. If the human intrusion is projected to occur more than 10,000 years after disposal, the dose analysis of the human intrusion case need not be presented in the TSPA-LA, only in an Environmental Impact Statement and the dose limits for the human intrusion standard would not apply.

In 10 CFR 63.322, a stylized human intrusion is specified that considers an “intruder” to be someone drilling a land-surface borehole using a drilling apparatus (under the common techniques and practices that are currently employed in exploratory drilling for groundwater in the region around Yucca Mountain). In the stylized analysis, it is specified that the intruder drills directly through a single degraded waste package and subsequently into the uppermost aquifer underlying the proposed repository. The intrusion then causes the subsequent compromise and release to groundwater of the waste in the penetrated waste package. Figure 4.4-1 provides a schematic of this stylized condition.

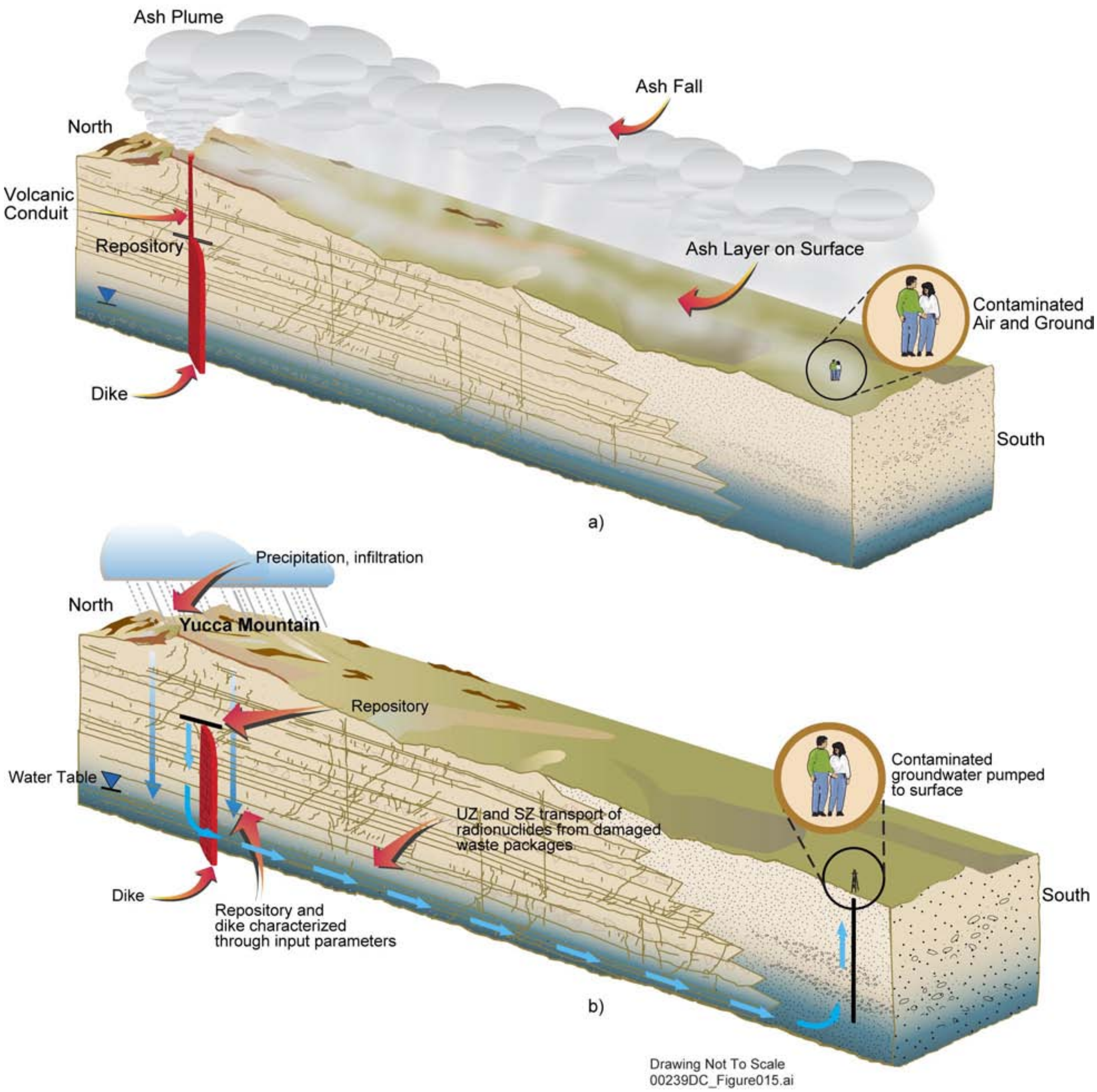
The compressive strength and ductility of the metals from which the drip shields and waste packages are fabricated differ significantly from the rock that would surround them (BSC 2001 [155950], Appendix A). Drillers would notice these differences. For example, the drilling assembly is expected to buckle and bend when the bit attempts to penetrate the titanium drip shield and waste package (drill bits that are designed for rock do not easily penetrate metal, particularly titanium). The drillers should, therefore, recognize that they have attempted to drill into some material other than rock for at least as long as the drip shield or waste packages are intact. Analyses predict that the first failures of the waste package material, Alloy 22, due to general corrosion occur after approximately 30,000 years (BSC 2001 [155950], Appendix A). Therefore, the earliest time a human intrusion could occur without recognition by a driller is 30,000 years. Consequently, documentation of the human intrusion stylized analysis in the TSPA-LA will be limited to a description of the technical basis and analyses to support the determination of the time of occurrence of the human intrusion. This will be conducted and documented external to the TSPA-specific documentation (e.g., in a Waste Package AMR).

Because the dose from the human intrusion is expected to occur after the 10,000-year regulatory compliance period, dose analysis of the stylized human intrusion case is not required for TSPA-LA. Instead, the human intrusion dose analysis is presented in *Final Environmental Impact Statement for a Geologic Repository for the Disposal of Spent Nuclear Fuel and High-Level Radioactive Waste at Yucca Mountain, Nye County, Nevada* (DOE 2002 [155970]) in accordance with 10 CFR 63.321(b)(2). Details of this analysis are documented in the *TSPA-FEIS Report* (Williams 2001 [157307], Section 6.4) and is based on prescribed assumptions about the human intrusion stylized analysis given in 10 CFR 63.322.



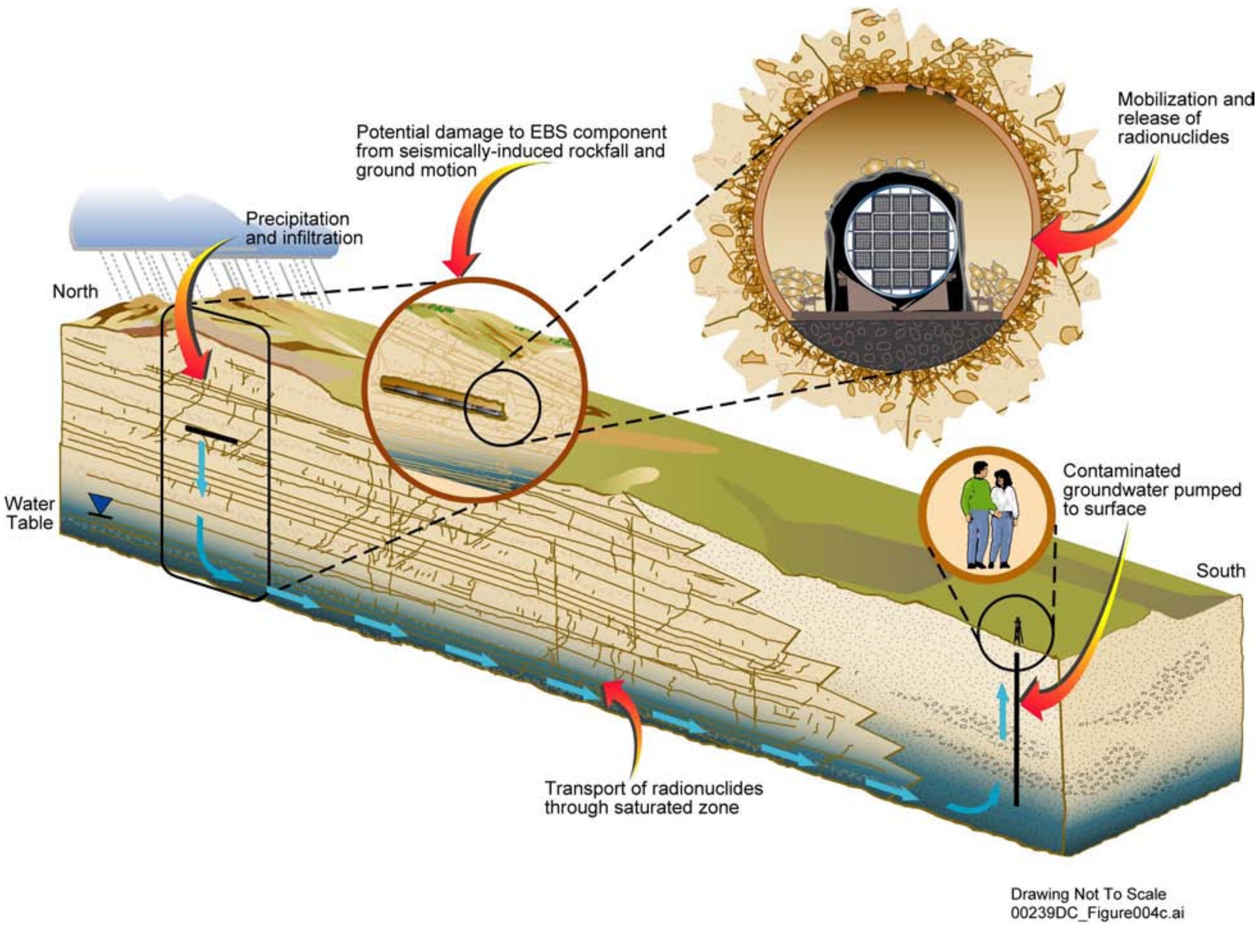
Source: Modification of DOE 2002 [156958], Figure 3-17

Figure 4.1-1. Schematic Illustration of the Components of the Nominal Scenario Class



Source: Modification of BSC 2001 [156958], Figure 3-67

Figure 4.2-1. Schematic Illustration of the Igneous Scenario Classes Two Modeling Cases: a) Volcanic Eruption, and b) Igneous Intrusion



Source: Modification of DOE 2001 [155734], Figure 3-64

Figure 4.3-1. Schematic Illustration of the Seismic Scenario Class

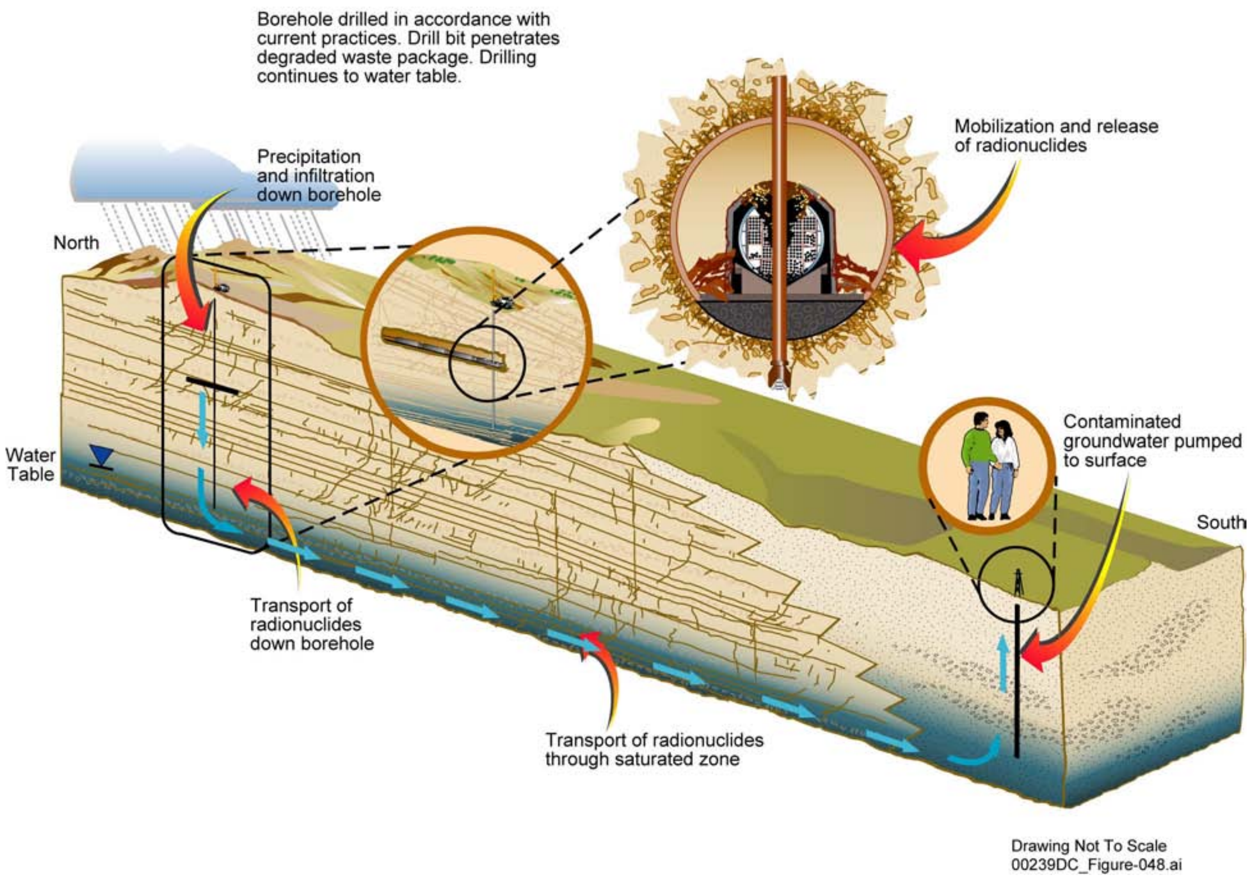


Figure 4.4-1. Schematic Illustration of the Stylized Human Intrusion Analysis

5. TSPA-LA MODEL COMPONENTS

Eight principal model components in the TSPA-LA model will be combined to evaluate the proposed repository system performance for nominal and disruptive event scenario classes. The purpose of this section is to provide an overview of the individual model components and model architecture for the TSPA-LA model and outline how these models will be implemented for the three scenario classes. As noted in the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]), the model abstraction review process ends with a review of how the abstracted models are implemented in the TSPA model. This section provides information to facilitate this review and in particular describes how the models from different parts of the repository system are integrated together.

Figures 5-1 through 5-5 depict the general flow of information for the principal model components and scenario classes of the TSPA-LA. The model components, listed in the general order information is passed from model to model, include:

- Unsaturated zone flow
- Engineered barrier system environment
- Waste package and drip shield degradation
- Waste form degradation and mobilization
- Engineered barrier system flow and transport
- Unsaturated zone transport
- Saturated zone flow and transport
- Biosphere.

The scenario classes include the nominal (undisturbed) scenario class and the disruptive event scenario classes.

Nominal Scenario Class–The nominal scenario class exercises the model components to describe the anticipated sequence of processes that are likely to occur during the lifetime of the proposed repository (i.e., those with a probability of occurrence of close to one).

Disruptive Event Scenario Classes–The two disruptive event scenario classes exercise the model components to describe the sequence of events and processes that, if they occur, could have a significant consequence to public health, but whose probability of occurrence is very small. These classes consider volcanic eruption, igneous intrusion, and seismic ground motion and fault displacement (if screened in) as events that have low probability of occurrence during the time period of evaluation.

The igneous scenario class includes (1) igneous intrusion resulting in indirect releases via groundwater, and (2) volcanic eruption resulting in direct releases via ash dispersal and deposition.

The seismic scenario class includes seismic ground motion and fault displacement (if screened in) resulting in indirect releases via groundwater.

The nominal and disruptive scenario classes together contribute to the expected annual dose (Figure 5-1). Figures 5-2 to 5-5 show the individual flow-of-information wheels for the nominal scenario class, the two igneous disruptive modeling cases, and the seismic scenario class. These figures provide a visualization of how information flows between principal model components within each of the scenario classes and modeling cases. Note that the nominal, igneous intrusion, and seismic modeling cases utilize many of the same models and parameters, so these wheels look very similar.

An outline of the following sections is as follows. Section 5.1 describes the individual model components along with their key inputs and outputs. The model components for TSPA-LA will be similar to those described in the *SSPA Volume 1* (BSC 2001 [155950]), *SSPA Volume 2* (BSC 2001 [154659]), and *TSPA-FEIS Report* (Williams 2001 [157307]). The section also presents a table summarizing the updates planned for the LA model. Section 5.2 provides an overview of how information flows between the models and the computer code architecture that facilitates the information flow. Section 5.3 describes the implementation of the three scenario classes: nominal, igneous, and seismic.

5.1 MODEL COMPONENTS

The TSPA-LA model components will be similar to the TSPA-SR and TSPA-FEIS model components with differences resulting primarily from improved quantification of uncertainties, incorporation of new information and understanding, and developments to address KTI agreements and improve technical bases. The project made many of these improvements during the *SSPA* (BSC 2001 [155950]; BSC 2001 [154659]) and for the *TSPA-FEIS Report* (Williams 2001 [157307]), and much of the work since then has focused on quality assurance and validation of these models. The principal TSPA-LA model components (UZ Flow, Engineered Barrier System (EBS) Environment, Waste Form Degradation and Mobilization, Waste Package and Drip Shield Degradation, EBS Flow and Transport, UZ Transport, SZ Flow and Transport, and Biosphere) and their supporting submodels are illustrated in Figure 5.1-1. The principal model components are in the top row of the figure, with submodels pictured below the principal model component level. Submodels represent a further division of the principal model components. Note that submodels have arrows on the left side illustrating links to the parent model component. Arrows on the right side of submodels illustrate input feeds from submodels of other principal model components. Only those models that provide direct input to the TSPA model are shown. Figure 5.1-1 also illustrates the Disruptive Events models (i.e., nominal model components plus the atmospheric transport model for volcanic eruption modeling case, and repository level impacts depending on the disruptive event under consideration).

Potential key updates to the TSPA-FEIS model for the LA model for each component are summarized in Table 5.1-1. The models are all part of the TSPA-LA model, and run in the GoldSim model framework. Note, model changes may include revised model input and output distributions and changes to mathematical models. These changes should improve representation of important processes and uncertainty at the principal model component level and in the TSPA-LA model. Also, note that there are no key model changes planned in saturated zone flow and transport. A description of the hierarchy of major documents for each TSPA-LA model component and their submodels is provided in Appendix G. The document hierarchy is shown in Figures G-1 through G-10. The models and their corresponding model reports are listed in Table G-1. Appendix G, as noted in Section 1, is an evolving plan for document development, and thus does not contain DIRS numbers or references. Nearly all of the TSPA-FEIS model components will be updated and improved for the TSPA-LA, some more than others.

Table 5.1-1. Summary of Potential Key Model Changes from TSPA-FEIS to TSPA-LA

TSPA Model Component	Submodel	Description of Changes
UZ Flow	Mountain-Scale Flow	Changes in UZ flow grid to accommodate changes in repository layout and increased resolution in the repository area. Number of grid points increases from 100,000 to 250,000. The number of flow fields may increase to improve treatment of uncertainty in flow fields due to fraction of flowing fractures.
	Seepage	Data from long-term liquid-release experiments will be incorporated to reduce the estimation uncertainty in seepage-relevant parameters and obtain estimates for the previously untested lower lithophysal zone of the Topopah Spring Tuff unit. An updated distribution of the flow-focusing factor for seepage is expected to be implemented that is based on simulations of unsaturated-zone flow using heterogeneous permeability fields. Will change response surface for ambient seepage to be a function of underlying physical parameters such as permeability and fracture alpha. Will develop a new and separate response surface for the thermal period (approximately first 2000 years of simulation period).
EBS Environment	Thermal Hydrologic Environment	The model for thermal properties of the host rock is expected to be updated to integrate new information obtained for the Topopah Spring lower lithophysal unit and to account for uncertainty and spatial variability of thermal properties. Model is expected to be revised to incorporate waste package loading sequence and variable (temporal and spatial) ventilation efficiency. Location of percolation flux above drift for input to seepage model is expected to change based on new UZ flow model analyses. Cold-trap effect (drift-scale condensation) and drip-shield condensation are expected to be included if they cannot be screened out from TSPA-LA model.
	Chemical Environment	The model will improve the representation of evolution of solids and water during the thermal period due to evaporation and deliquescence of water occurring in the emplacement drifts. Additional anions and cations are expected to be added to accommodate analysis and modeling of waste package localized corrosion. Sorption (K_ds) in the invert will be set to zero.

Table 5.1-1. Summary of Potential Key Model Changes from TSPA-FEIS to TSPA-LA (Continued)

TSPA Model Component	Submodel	Description of Changes
Waste Package and Drip Shield Degradation	Waste Package/Drip Shield Degradation (WAPDEG)	**Stress Corrosion Cracking (SCC) of Alloy 22** Will update representation for the fraction of weld flaws in waste packages that can propagate through wall thickness by SCC. The value for repassivation slope at SCC crack tip is expected to be updated. The representation of uncertainty in the residual stress profile for the closure weld region of the outer waste package barrier is expected to be improved. The representation of uncertainty in the residual stress profile for the closure weld region of the inner waste package barrier is expected to be improved. The distribution of the threshold stress for crack initiation is expected to be updated. SCC initiation at preexisting flaws is expected to be modeled with the more conservative of the threshold stress and threshold stress intensity approaches. **General Corrosion** The TSPA-LA model is expected to take into account temperature dependence of the general corrosion rate of the Alloy 22 outer waste package barrier. **Localized Corrosion** Localized corrosion model is expected to include additional dependency on chemical environment.
	Igneous Waste Package Damage Model	Model is expected to be developed to define extent of waste package damage due to deleterious chemical and physical environments.
Waste Form Degradation and Mobilization	Radionuclide Inventory	An updated radionuclide screening analysis using new screening criteria is expected to introduce new radionuclides into groundwater dose (e.g., Cs-135).
	In-Package Chemistry	The model is expected to be updated to take into account the effect of waste form and iron degradation products on in-package chemistry. A time-dependent function for water volume in package is expected to be developed.
	Cladding Degradation	The model is expected to incorporate new probability distributions for creep rupture and stress corrosion cracking parameters. Unzipping model is expected to be eliminated. Localized corrosion perforation rate is expected to be based on chlorides and ferric chlorides. Modification of model for failure due to seismic ground motion and implementation in seismic scenario is expected.
	Waste Form Degradation Rate	No major changes planned.
	Dissolved Concentration Limits	Model is expected to be modified to increase the range for the uncertainty in the effect of the controlling mineral phases for plutonium, neptunium, and thorium and to account for the effects of colloids.
	Colloids	Commercial spent nuclear fuel (CSNF) and/or DOE spent nuclear fuel (DSNF) colloids are expected to be added.
	Igneous Impact on Waste Form	Current cladding, in-package chemistry, waste form degradation and solubility models are expected to be modified to account for the effects of igneous intrusion.

Table 5.1-1. Summary of Potential Key Model Changes from TSPA-FEIS to TSPA-LA (Continued)

TSPA Model Component	Submodel	Description of Changes
EBS Flow and Transport	EBS Flow	May develop model to predict area of waste package surface dripped on as a function of in-drift seepage and drip shield degradation to accommodate localized corrosion model needs.
UZ Transport	Drift Shadow Transport	Diffusive coupling between EBS and UZ is expected to be modified.
	UZ Transport Model	Modify FEHM particle tracker matrix diffusion approach.
Biosphere	Biosphere	New eruptive biosphere dose conversion factor (BDCF) models will be implemented, consisting of an improved inhalation modeling component and a steady-state component. Also, groundwater protection dose will be based on FGR-11 (Eckerman et al. 1988 [101069])
Disruptive Events	Seismic Scenario Model	New model is expected to be developed and implemented to determine release resulting from ground motion and fault displacement (if screened in) and subsequent potential damage to drip shield, waste package, and cladding.
	Igneous Scenario Model	Several model parameters are expected to change for both eruption and intrusion modeling cases including wind speed, number of conduits intersecting drifts, and vent probability. Number of waste packages impacted by igneous intrusion event is expected to be based on process model analyses that will delineate two primary zones in a drift. Zone 1 will contain complete waste package destruction and Zone 2 will contain an aggressive corrosion of Alloy 22 during intrusive event and possible mechanical disruption of waste package. Tephra redistribution model is expected to be added to the eruptive scenario.

Model components and submodels illustrated in Figure 5.1-1 are described in the following sections. Note that submodels have arrows on the left side illustrating links to the parent model component. Arrows on the right side of submodels illustrate input feeds from submodels of other model components. The documentation hierarchy supporting the development of principal model components and their submodels is presented in Appendix G, both graphically and in tabular form. Note that the diagrams presented in Appendix G reflect how information flows between the supporting documentation. This flow of information between documents may be discretized differently than the flow of information between models as depicted in Figure 5.1-1. In the former case, the information flow supports model development and analyses, whereas in the latter case information flow enables model implementation.

Unsaturated Zone (UZ) Flow

The UZ flow model component will define the temporal and spatial distribution of water flow through the unsaturated tuffs above and below the proposed repository horizon and the temporal and spatial distribution of water seeps into the waste emplacement drifts. The UZ component of the TSPA includes five submodels of flow in the UZ:

- Climate
- Infiltration
- Mountain-scale UZ water flow
- Drift seepage
- Drift-scale coupled processes

A brief description of these submodels is provided below. See Table 5.1-1 for a summary of potential UZ submodel changes from TSPA-FEIS to TSPA-LA.

Climate refers to the meteorological conditions that characteristically prevail in a particular region. Climate conditions at Yucca Mountain must be known to determine the hydrology within and around Yucca Mountain. The climate submodel will provide future histories of the following output variables.

- Precipitation and air temperature will serve as inputs to the infiltration submodel.
- Water table rise for future climates will serve as a bottom boundary condition for the mountain-scale UZ flow model and the thermal hydrologic models.
- The climate and infiltration models will also be used to scale changes in SZ groundwater flux for future climates to the SZ flow and transport models.

The climate model is formulated using paleoclimate and paleoenvironmental reconstructions based on microfossil evaluations in Owens Lake cores and calcite isotope records from Devil's Hole. The sequence and duration of past climate periods are identified from the records and applied to the Yucca Mountain site, which has a similar climate setting. The temperature and precipitation records of present-day meteorological stations at colder and wetter sites are selected to represent future climate states. In addition, paleohydrologic data (e.g., paleospring deposits) are used to estimate how the water table fluctuates with climate. Water table changes, plus calculated infiltration changes, will be used to estimate changes in SZ groundwater flux for future climates.

The infiltration submodel provides net infiltration of meteoric water at the surface, which will be used as a top boundary condition for the mountain-scale-flow submodel and the multi-scale thermal-hydrologic (MSTH) submodel (a submodel in the EBS environment model). Net infiltration is the penetration of water through the ground surface to a depth where it can no longer be withdrawn by evaporation or transpiration by plants. Infiltration occurs once water has entered bedrock or has penetrated below the root zone in soil. The main components of net infiltration are precipitation, evapotranspiration (evaporation plus transpiration), and surface-water runoff and run-on. These components will be incorporated into a watershed-scale, volume-balanced model using a snowpack submodel, an evaporation and net radiation submodel, one-dimensional (vertical) root-zone infiltration submodels, and a two-dimensional surface-water, flow-routing submodel (CRWMS M&O 2000 [151940], Section 3.5).

UZ water flow refers to the percolation of groundwater through rocks above the water table. The mountain-scale UZ flow model provides flow fields (spatial distributions of fracture and matrix saturations and percolation fluxes) to the UZ radionuclide transport model. This model is based on a steady-state moisture flow assumption, a volume-averaged modeling approach with dual-permeability model representation of fractures and tuff matrix, and a multilayer three-dimensional grid block approximation, with each hydraulic unit characterized by averaged and calibrated rock properties. Calibrated property sets will be developed for upper-bound, mean, and lower-bound infiltration rates of the modern (present-day) climate, to match observed ambient conditions of matrix liquid saturation, water potential and temperature data, perched water data, pneumatic data, and geochemical data. Major faults will be included in the model explicitly. In fault zones, fracture density and permeability are higher than in the rest of the model, which enables them to act as preferential flow paths in parts of the model. The mountain-scale UZ flow model will also provide calibrated sets of hydrologic properties to the seepage and thermal hydrologic models.

Seepage is the movement of liquid water into emplacement drifts. The seepage submodel provides seepage flux into the drifts during thermal and ambient periods. Seepage flux will be used by the EBS Environment and EBS Flow and Transport TSPA model components. The seepage submodel requires percolation flux as input and this input is expected to be provided by the MSTH model.

Heat input from radioactive decay drives coupled chemical processes. Boiling and resultant precipitation of naturally occurring minerals may result in the reduction of fracture apertures. Regions in which condensate waters accumulate and then readily flow may result in dissolution and precipitation of minerals, potentially increasing fracture apertures in one location while reducing them in another. These processes may also influence the water chemistry entering the emplacement drifts. The Drift-Scale Coupled Processes model will be used to provide boundary conditions for EBS chemical environment simulations. This model will represent the thermally driven evolution of water chemistry and gas composition in the near-field host rock over time. This model abstracts results from a fully coupled two-dimensional thermal-hydrologic-chemical (THC) chimney model that will be applied at two representative locations in the proposed repository, one in the lithophysal unit and one in the non-lithophysal unit. Abstraction results will be in the form of response surfaces and used in chemical environment model simulations to represent time-dependent water and gas compositions that enter the emplacement drifts located in each of these units.

It is important to note that the UZ flow models do not include potential effects of changes in the hydrology induced by disruptive events (e.g., seismic and igneous events). The justification for excluding these disruptive events will be documented through the FEP screening process.

EBS Environment

EBS environments refer to the thermal-hydrologic and chemical environments within the emplacement drifts. These environments are important to proposed repository performance because they help determine degradation rates of the engineered barrier components, quantities and species of mobilized radionuclides, and transport of radionuclides and fluids through the drift into the UZ. Table 5.1-1 summarizes potential EBS environment model changes from TSPA-FEIS to TSPA-LA.

Heat from the waste form will strongly influence local conditions around the waste packages and within the drifts. The thermal-hydrologic environment in the emplacement drifts depends on the decay-heat characteristics of the individual waste packages. The in-drift thermal-hydrologic environment for TSPA simulations will be computed using the MSTH model. This model quantifies processes such as lateral heat losses associated with proximity to repository edges, spatially and temporally (e.g., because of climate changes) variable infiltration rates, waste emplacement in different host rock units, in-drift heat transfer effects, and waste packages.

The MSTH model will provide temperature, relative humidity (RH), liquid saturation and flow rate, and liquid evaporation rate at several in-drift locations. These results will serve as inputs to chemical environment, EBS flow and transport, waste package and drip shield degradation, and waste form degradation and mobilization models. The MSTH model is expected to provide percolation flux to the seepage submodel for the thermal and ambient periods.

Inputs to the MSTH model will come from a variety of sources. The hydrologic property data sets developed for the UZ flow model will also be applied to the MSTH model. There will be calibrated mountain- and drift-scale property sets for low, nominal, and high infiltration rates and for flow around and flow through the perched water zones below the repository. The calibrated drift-scale property sets will be applied to the MSTH model. Repository design specifications needed as input include mass loading, repository layout, and heat output over time.

The purpose of the chemical environment model is to provide a quantitative description of the major time-dependent chemical compositional parameters required by the drip shield and waste package degradation models, the waste form dissolved concentration submodel, and EBS radionuclide transport model. In particular, this model will determine the aqueous solution compositions and types of precipitates (including salts) that may form as water is evaporated within the drift. The model will assess the effects on water chemistry of accumulated precipitates, the effects of heat and RH on water vapor condensation, and the dissolution of precipitates/salts previously deposited on drip shield, waste package, and other EBS component surfaces. The evaluation will include changes in aqueous solution compositions resulting from evaporation driven by temperature gradients within the drift (e.g., from package surface to drift wall) and from interactions with grout.

Several processes and interactions among in-drift gas, water, and EBS components potentially affect the in-drift chemical environment. The chemical environment model is based on the following results and interpretations:

- Water and grout interactions–The effect on water chemistry of chemical reactions between water that enters the drift and grout materials used to stabilize rock bolts.
- Salts precipitation and salts dissolution–The types of precipitates that may form as water is evaporated within the drift.
- Deliquescence–The types of aqueous solutions that may form due to deliquescence by salt precipitates and small dust particles.

- Microbial activity and effects–The ultimate abundance of microbes within the drift environment is estimated (bounded) based on nutrient and energy limitations within the drift.
- Corrosion and degradation of EBS components–This submodel will evaluate changes to water chemistry resulting from chemical reactions between the aqueous seepage that enters the drift and metallic components and their corrosion products encountered along the flow paths.

Results of chemical environment model simulations will be incorporated in the TSPA-LA model as abstracted EBS fluid composition response surfaces for various regions of the EBS. These response surfaces will set the chemical environment within the GoldSim EBS cells. By coupling time histories of chemical environment compositional parameters to each cell environment, the chemical environment model will be effectively coupled to the waste package degradation model, waste form mobilization model, and EBS transport model.

The chemical environment model will have several connections with other TSPA model components. This model takes input from the UZ seepage model, UZ drift-scale coupled processes model and the EBS thermal-hydrologic model and provides output to the drip shield and waste package corrosion models, the waste form degradation and mobilization model (degradation, radionuclide solubility, colloid stability), and EBS transport.

Waste Package and Drip Shield Degradation

The waste package and drip shield together form the primary component of the EBS. The TSPA-LA model component for evaluating degradation of the waste package and drip shield is the WAste Package DEGradation (WAPDEG) model. WAPDEG is based on a stochastic simulation approach and provides a description of waste package and drip shield degradation, which occurs as a function of time and proposed repository location for specific design and thermal-hydrologic-chemical exposure conditions. Table 5.1-1 summarizes potential waste package and drip shield degradation model changes from TSPA-FEIS to TSPA-LA. Several degradation processes potentially affect waste package and drip shield performance. WAPDEG integrates and relates submodels that provide results and interpretations for the following degradation processes:

- Humid-air general corrosion, a relatively uniform thinning of materials, occurs when the RH at the surface of the drip shield and waste package in the emplacement drift exceeds a threshold value.
- Aqueous general corrosion, a relatively uniform thinning of materials, occurs when a material surface is wetted, as from seepage or drips.
- Localized corrosion is induced by local variations in the electrochemical potential or driving force for corrosion on a micro-scale over small regions.
- Stress corrosion cracking (SCC) is a crack propagation process caused by the combined and synergistic interaction of mechanical stress and corrosion reactions.
- Microbially-induced corrosion is caused by the metabolic activity of microorganisms.

- Thermal aging and phase instability is caused by prolonged exposure to elevated temperature environments, resulting in microstructure changes of waste package and drip shield materials, potentially changing their corrosion behavior, such as by enhancing general corrosion.
- Manufacturing and material defects, including defects due to improper heat treatment, can augment corrosion processes and result in early failure of waste packages.

These degradation processes are a function of the material properties of the drip shield and waste package, and the sequence of events that is anticipated to occur subsequent to repository closure. Three main types of degradation will be considered directly: humid-air general corrosion, aqueous general corrosion, and SCC. Two additional corrosion processes, microbially-induced corrosion, and thermal aging and phase instability, will be considered to enhance general corrosion on the waste package. Localized corrosion will be evaluated for the predicted environmental conditions in the proposed repository, and may be implemented in the TSPA-LA, if necessary.

A key input to the SCC model is information regarding defects, incipient cracks, and manufacturing defects. Preexisting manufacturing flaws in the closure lid welds are the most likely sites for SCC failure. The frequency and size distributions for manufacturing flaws in the closure welds will likely be based on relevant published data such as data for stainless steel pipe welds in nuclear power plants.

The primary models supplying input to drip shield and waste package degradation abstractions are the EBS environment models and the in-package chemistry model. Inputs to the drip shield degradation model will consist of emplacement drift temperature and RH profiles as a function of time. Inputs to the waste package degradation model consist of: emplacement drift temperature and RH profiles as a function of time, chemical composition of gases and dripping water, mineral deposits (precipitates and salts), and in-package chemical conditions.

In addition, the waste package/drip shield models will be coupled to disruptive scenario class models (e.g., rockfall, igneous intrusion, and seismic) if it is found necessary to determine waste package and drip shield lifetimes under these conditions.

Output from the drip shield and waste package degradation models will be a time-dependent quantitative assessment of the drip shield and waste package degradation and failure. Results will include: the time to initial breach for the drip shield and the waste package; time to first breach of the waste package by stress-corrosion crack failure; and the degree of drip shield and waste package failure as a function of time. The time of the first breach of the waste package corresponds to the start of waste form degradation within the breached package.

The processes leading to early waste package failure are under evaluation as well, and may result in an early waste package failure model for TSPA-LA.

Waste-Form Degradation and Mobilization

The purpose of the waste form degradation and mobilization model is to evaluate the rate of degradation of cladding and waste matrix, the dissolved concentration of radioisotopes, and the migration of radioisotopes through remaining portions of the waste package. Specifically, the waste form degradation and mobilization model consists of the following submodels that:

- Provide the radionuclide inventory
- Evaluate in-package water chemistry (In-Package Chemistry Abstraction)
- Evaluate the rate of Zircaloy cladding degradation (for CSNF) (Clad Degradation Abstraction)
- Evaluate the matrix degradation rates for CSNF, DSNF, and high-level radioactive waste (HLW) waste forms (Waste Form Matrix Degradation Abstractions)
- Evaluate the radionuclide concentrations for aqueous phases (Dissolved Radionuclide Concentration Abstraction)
- Evaluate the waste form and EBS colloidal phases (Colloidal Radionuclide Concentration Abstraction).

Table 5.1-1 summarizes potential waste form degradation and mobilization model changes from TSPA-FEIS to TSPA-LA.

The waste form degradation and mobilization model for TSPA-LA will be applicable to three generic waste form categories: (1) CSNF, (2) DSNF, and (3) HLW glass. These three categories are contained and disposed of in two types of waste packages—CSNF waste packages and codisposal waste packages, with the latter containing both DSNF and HLW glass. As was done in the TSPA-SR, releases from naval spent nuclear fuel (SNF) will be conservatively represented by CSNF releases.

For both the CSNF and codisposal waste packages, the waste form degradation model will describe the evolution of the chemical environment in the packages, corrosion of the protective cladding leading to perforations and cladding failure in the case of CSNF, dissolution of the exposed fuel matrix, and mobilization of the radionuclides. The calculated radionuclide release rates from waste forms will, in turn, be provided to the EBS flow and transport model, which will calculate the radionuclide releases from the EBS.

The waste form degradation and mobilization model for CSNF, DSNF, and HLW is primarily designed for the nominal scenario class but will also be used as a source term for the igneous and seismic scenario classes. The submodels will be computationally linked in a sequential manner. The submodels are described in the following paragraphs.

The model abstraction for the waste inventory defines the source term for the CSNF and codisposal waste packages in terms of both the quantity and spectrum of radioisotopes. This information will be used with the abstraction for waste form degradation to determine the mobilization of the radionuclides. The computer implementation of the inventory abstraction will be a simple table lookup of the quantity of radionuclides at the time of waste emplacement for the CSNF and codisposal waste packages.

The in-package chemistry component will model the evolution of the water chemistry inside the failed waste package as a function of water inflow rate and waste package and waste form corrosion rate. The water chemistry characteristics of importance will primarily be pH, ionic strength, and total carbonate concentration. Additional chemistry characteristics may include concentrations of fluoride and chloride and partial pressure of oxygen and carbon dioxide. This water chemistry information will be used by five other waste form degradation and mobilization submodels, which will be dependent on the in-package water chemistry. Specifically, the waste-form matrix degradation rate for CSNF and HLW, the dissolved concentration of radioisotopes, stability of colloids, and degradation of CSNF cladding will be dependent on water chemistry parameters. As was done in the TSPA-SR, the DSNF degradation rate is expected to be represented by a constant rate independent of chemistry changes.

The cladding degradation component determines the fraction of fuel rods in the CSNF waste packages with perforated cladding as a function of various failure mechanisms induced by physical and chemical processes. Because these mechanisms vary with time, the rate at which the rods fail (by perforation) will determine the rate at which the CSNF waste matrix is exposed to water. Cladding failure mechanisms include: initial perforations within the reactor or during storage, perforations from creep when in dry storage (or disposal at high temperatures) or stress corrosion cracking (SCC) from high stress when temperatures are 300ºC or greater, perforations as a result of ground motion and accelerations induced by an earthquake, and perforations from localized corrosion as a result of halogen anions (e.g., fluoride or chloride) inside the waste package.

The waste form matrix abstraction will estimate the rates at which the CSNF, DSNF, and HLW forms dissolve as a function of the inflow conditions and in-package chemistry. The abstractions for waste form degradation are based on laboratory data obtained under various flow conditions. The DSNF have multiple waste types that will be grouped into 10 groups for the purposes of the TSPA analyses, similar to what was done for the SR, except that naval SNF will not be included as one of the groups. These DSNF groups will be compared with the bounding case utilized in the TSPA-LA in a series of sensitivity analyses (see Appendix E, Section E.5). Naval SNF will be compared with CSNF as a sensitivity analysis.

The dissolved radionuclide concentration submodel provides the radionuclide solubilities that will be used in the release calculations. This submodel will be applied in both the waste package and invert.

The function of the waste form and EBS colloidal radionuclide concentration submodel is to calculate the concentration of colloid-associated radionuclides. Colloid transport is potentially important for radionuclide elements that have low solubility and can be entrained in, or sorbed onto, waste form, engineered barrier, or geologic barrier materials that form colloidal particles. Three major types of colloids, based on the source of the colloid substrate material, are recognized to be important, waste form colloids, corrosion-product colloids, and groundwater colloids.

Key inputs to the waste form degradation and mobilization models will include (1) a set of initial materials within the waste package and their major element composition and thermodynamic/kinetic coefficients, (2) time-dependent water fluxes in the drift provided by the EBS flow submodel, and (3) waste package temperatures provided by EBS thermal-hydrologic environment submodel (MSTH).

EBS Flow and Transport

The primary goal of the EBS flow and transport component is to calculate the rate of radionuclide release from the EBS to the UZ. This quantity is determined by seepage, the presence of water films, drip shield and waste package degradation, cladding and waste form degradation, EBS thermal and chemical environments, and the design of the EBS.

The EBS radionuclide flow and transport submodel will include one-dimensional advective and diffusive transport, as well as retardation due to sorption and precipitation. This model will be input directly into the TSPA model and will make use of the compartment or cell modeling capability within GoldSim. Note that there are no submodels for this component in Figure 5.1-1 as this model is implemented directly in GoldSim. Table 5.1-1 summarizes potential EBS flow and transport model changes from TSPA-FEIS to TSPA-LA.

The radionuclide transport pathway from the waste form, downward to the edge of the EBS (i.e., the interface between the drift wall and the UZ) beneath the waste packages, will be defined, using GoldSim cells arranged vertically. Implementation will include the following aspects:

- The EBS water flow submodel will define the amount of flow at a number of locations in the drift, including through the drip shield, the waste package, and the invert.
- Diffusive transport will be modeled from the waste form to the waste package outer barrier through thin films on internal structures within waste packages.
- Sorption of radionuclides on corrosion products from internal waste package structures will be considered.
- The invert will be comprised of a granular material that will act as a diffusive barrier.
- The bottom boundary condition for the GoldSim implementation of the transport model will be established based on continuity of radionuclide concentration and flux exiting the drift and entering the UZ.

The EBS flow submodel has three major inputs. The first input is the drift seepage submodel that defines the fluid flux into the EBS as a function of time, location within the proposed repository, and climate state. The second input is the drip shield and waste package degradation model that defines the type, number, and timing of breaches in these components. The third input is the abstraction of the thermal-hydrologic response of the EBS environment that defines the time-dependent temperature, RH, and evaporative fluxes in the EBS.

The EBS transport submodel has four major inputs. The first input is the output from the EBS flow abstraction that defines the fluid fluxes through the waste package and invert as a function of the time-dependent conditions in the EBS. The remaining inputs are the waste form dissolution rates, radionuclide solubility limits, and colloidal concentrations that are required to define the mobilized concentration of radionuclides for advective and diffusive transport.

UZ Transport

The UZ radionuclide transport component calculates the migration of radionuclides from the EBS of the proposed repository, through the UZ, to the water table. Consistent with the mountain-scale flow model, the UZ transport model will use a dual continuum model in which fracture and matrix transport are coupled through advective and diffusive transport mechanisms. Transport from the repository to the water table will be calculated in three-dimensions using the FEHM computer code. The FEHM particle tracking algorithm simulates aqueous-phase and colloid-facilitated radionuclide transport processes through the UZ, including:

- Advective transport (within and between fracture and matrix continua), which is the movement of dissolved or colloidal material along with the bulk flow of water. In many of the hydrogeologic units, advection through fractures is expected to dominate transport behavior.
- Hydrodynamic dispersion, which refers to the spreading of radionuclides as they transport, caused by localized variations in the flow field and by diffusion.
- Matrix diffusion, which is the movement of dissolved or colloidal material in the matrix from a zone of high concentration to a zone of low concentration
- Sorption, which is the uptake of radionuclides by the solid rock in contact with water containing dissolved radionuclides.
- Radionuclide decay, which is the spontaneous breakdown or disintegration of radionuclides.

The UZ transport component will be incorporated into TSPA-LA in the same manner as was done for the TSPA-SR and TSPA-FEIS, that is, by coupling the transport model directly to the TSPA model. As in the TSPA-SR, probability distributions will be sampled for key uncertain input parameters. Table 5.1-1 summarizes potential UZ transport model changes from TSPA-FEIS to TSPA-LA.

An important improvement to the UZ transport model component for TSPA-LA will be the drift-scale transport submodel. This submodel will better represent the transport conditions beneath the emplacement drifts. Flow in the UZ tends to be diverted by an opening such as an emplacement drift. This diversion leads to the absence of downward flow beneath the drift, which produces a shadow zone of reduced water flux and water saturation. As a result, radionuclide transport may be substantially delayed in the region underneath the drift.

The UZ radionuclide transport model will take as its input radionuclide mass flux from the EBS flow and transport model. Mountain-scale UZ flow fields (spatial distributions of fracture and matrix saturations and percolation fluxes) will transport the released radionuclides to the SZ. As its output, it will provide radionuclide mass flux at the water table to the SZ flow and transport model.

SZ Flow and Transport

The SZ flow and transport component of the TSPA-LA will be used to evaluate the migration of radionuclides from their introduction at the water table below the proposed repository to the point of release to the biosphere (e.g., water supply well). Radionuclides can move through the SZ either as solute (i.e., in the dissolved state) or associated with colloids (i.e., particles small enough to remain suspended indefinitely in water). For TSPA-LA, two models of SZ flow and transport will be used: a three-dimensional process level model that will be used to calculate flow fields and the transport of individual radionuclides important to dose, and a one-dimensional flow tube model that will be used to calculate the transport of daughter radionuclides (radionuclides that form by the decay of other radionuclides) of lesser importance.

The three-dimensional SZ flow and transport model will be implemented outside of GoldSim using the FEHM computer program. Transport in the SZ will be modeled using a particle-tracking method. In concept, particles will be released at a source point beneath the proposed repository into the flow field produced by the three-dimensional SZ flow model.

The three-dimensional transport model will not be used directly in the TSPA model. It will be used to perform a series of probabilistic transport simulations for a unit mass flux source to obtain breakthrough curves at 18-km. Transport simulations will produce a set of radionuclide mass unit breakthrough curves that will be used for TSPA-LA calculations. The convolution integral method will be used to quantify radionuclide transport to the biosphere. The convolution integral method will take a radionuclide source mass from the bottom of the UZ transport model for a given time step, and combine it with the appropriate breakthrough curve for that radionuclide, giving the masses and times that the radionuclides reach the 18-km boundary. The method will be implemented for TSPA-LA using numerical integration over the time of interest. Changes in recharge associated with climate variations will be approximated as a step from one steady-state flow condition to the next. The principal output of the convolution integral method will be the mass flux (as a function of time) at the 18-km boundary for each radionuclide and for each realization.

For some of the daughter radionuclides considered in LA, a one-dimensional SZ transport model will be used to account for decay and ingrowth during transport. The one-dimensional model will be incorporated directly in the TSPA-LA model as a series of pipes.

The SZ flow and transport models (breakthrough curves and one-dimensional transport model) will receive input from three other models. These other models include (1) the climate model, (2) the infiltration model, which provides input to scale the groundwater flux for future climates, and (3) the UZ particle tracking model, which will provide the magnitude and distribution of radionuclide source terms.

The SZ flow and transport models will not be directly coupled to the EBS thermal-hydrologic model or to the disruptive scenario models. Consequently, the SZ models will neglect the effects of the temperature field generated by the repository decay heat and any potential changes in the hydrostratigraphy induced by seismicity and igneous activity. Justification for this approach is provided in FEPs analyses.

Biosphere

The biosphere component of TSPA-LA will be used to predict radionuclide transport in the biosphere and the resulting exposure of the RMEI if there is a release of radioactive material after closure of the proposed repository. Two basic mechanisms of radionuclide release to the biosphere will be analyzed: (1) through the SZ via groundwater usage, and (2) through the air in the event of dispersal by a volcanic eruption. These two release scenarios correspond to the two modes of radionuclide introduction into the biosphere.

The primary result of the biosphere modeling for TSPA-LA will be the construction of biosphere dose conversion factor (BDCF) distributions, for both the groundwater-release modeling case and the volcanic-ash-release modeling case. These BDCFs include ingestion, inhalation, and external exposure pathways. In the groundwater-release modeling case, the dominant pathway is the ingestion of contaminated water and foods, while for the volcanic-ash-release modeling case, inhalation is the most important pathway. Table 5.1-1 summarizes the proposed biosphere model changes from TSPA-FEIS to TSPA-LA.

The biosphere component will be incorporated into the TSPA-LA calculations by the following methodology:

1. The first step of the process involves the calculation of the BDCF distributions, which represent radionuclide-dependent annual dose per unit activity concentration in groundwater or in volcanic ash for the RMEI specified by the regulation.
2. The second step of the process incorporates the water-usage volume that is specified in 10 CFR 63.312 as 3,000 acre-feet per year (only applies to groundwater-release modeling case).
3. The third step is within the TSPA-LA model and involves the calculation of the amount of each radionuclide reaching the geosphere/biosphere interface in a given year (only applies to groundwater-release modeling case).
4. The fourth step involves converting the amount of each radionuclide into a concentration, by dissolving the entire amount into the water-usage volume (only applies to groundwater-release modeling case).
5. The fifth step is the calculation of the annual dose incurred by the RMEI. Annual doses are calculated in the TSPA model for all radionuclides under consideration.

The biosphere is the last component in the chain of TSPA-LA components and, thus, has no output coupling. Upstream from the biosphere, there are two connections: (1) for the nominal scenario class, seismic scenario class, and igneous intrusion groundwater transport modeling case, the biosphere is coupled to the saturated zone flow and transport model; and (2) for the volcanic eruption modeling case, the biosphere is coupled to the volcanic dispersal model.

5.2 TSPA-LA ARCHITECTURE

Information transfer between the various model components in Figure 5.1-1 is depicted in Figures 5.2-1a and 5.2-1b. These two figures give a general, schematic description of how information will flow in the TSPA-LA, showing the principal pieces of information that will be passed between various model components and their submodels. These figures and the information presented in Section 5.1 may need to be updated as the details of the models are finalized. The decoupling of physical and chemical processes into separate models and passing information between them is facilitated by a natural division of the proposed repository system into a series of sequentially linked spatial domains (e.g., the UZ between the ground surface and the emplacement drifts, waste package, host rock near the drift, UZ between the drift and the water table, SZ, and biosphere). This decoupling of processes and division into spatial domains will allow the TSPA-LA model architecture and information flow to function as a sequential calculation in which each spatially based model may be run in succession, with output from an upstream spatial domain serving as the input for the spatial domain immediately downstream. This division works particularly well for radionuclide transport, which is the primary consideration of the TSPA models. For example, the three transport models (EBS radionuclide transport, UZ radionuclide transport, and SZ radionuclide transport) work together, with output as "mass versus time" from each upstream model serving as the input of mass versus time for the model immediately downstream.

It is important to note that within the TSPA model, most engineered-system calculations are performed for a limited number of waste package locations. In the model, each of these locations is representative of a group of waste packages with similar environmental characteristics. Radionuclide releases, for example, are calculated for a representative waste package and then scaled up by the number of failed waste packages in the group. (Note that the waste packages in a group do not all fail at the same time, because additional variability is included in the waste package degradation calculation.)

For the TSPA-Viability Assessment (VA), waste package groups were based on physical location (six potential repository subregions), waste type (CSNF, codisposal waste, or DSNF), and seepage (either (1) always exposed to seepage, (2) exposed to seepage during the wettest two climates, (3) exposed to seepage only during the wettest climate, or (4) never exposed to seepage) (*Total System Performance Assessment-Viability Assessment Analyses Technical Basis Document* (CRWMS M&O 1998 [100371], Section 11.2.1.3). For the TSPA-SR and TSPA-FEIS, the waste package groups were based on infiltration and assigned to five "infiltration bins" rather than physical location, because radionuclide dissolution and release depend more directly on infiltration than on the location within the proposed repository (CRWMS M&O 2000 [153246], Section 3.3.2). The other two discriminators are similar to before, though with fewer subdivisions. The TSPA-LA currently plans to base waste package groups on infiltration as was done in the TSPA-SR (see the five infiltration bins in Figure 5.2-1a); however, other options are also being considered. One approach is being considered to make the process more transparent and permit improved representation of spatial variability in thermal-hydrologic-chemical processes within the emplacement drifts and to account for lithophysal/nonlithophysal differences in mechanical and chemical properties. The new binning procedure would subdivide the repository into five bins of approximately equal area based on values of percolation at the repository horizon that exists for the medium infiltration scenario during the glacial transition climate. The criteria for selecting the approach include ease of implementation in TSPA-LA, transparency of approach, and technical defensibility of approach.

The information flow and sequential calculation approach described above will be implemented directly for the nominal scenario class and altered slightly for disruptive event scenario analyses. The igneous intrusion modeling case will utilize many aspects of the nominal scenario class and simply overlay an intrusive event and its effects on the system, as characterized by its probability and physical properties (e.g., number of waste packages damaged by intrusion, extent of damage to waste packages). After these effects are incorporated into the model, releases will be handled as in the nominal scenario class. The seismic scenario class will also utilize many aspects of the nominal scenario class and will be implemented in similar fashion by modifying the number and damage state of waste packages damaged by shaking, rockfall and fault displacement (if screened in). The volcanic eruption modeling case will be implemented by disconnecting the groundwater transport link and calculating direct volcanic effects (i.e., radionuclides carried by ash plumes from volcanic eruptions) using the code ASHPLUME directly linked to GoldSim.

The overall information flow and sequential calculation approach will form the basis for the architecture of the TSPA-LA computer code. The executive driver program, or integrating shell, that will link all the various component codes is GoldSim. GoldSim is a probabilistic sampling program that will tie all the model components, codes, and inputs/outputs together in a coherent structure that will allow for consistent parameter sampling among the model components. The GoldSim program will be used to conduct either single- or multiple-realization runs of the system. The multiple realization runs will yield a probability distribution of annual dose in the biosphere that will show uncertainty in annual dose based on uncertainty in all the model components.

Because of the need to conduct multiple realizations of the total system behavior, GoldSim is generally designed to model various components in a simplified fashion. The four ways that model components may be coupled into GoldSim, from most complex to least complex, include the following:

- External function calls to detailed process software codes (e.g., UZ transport software or waste package degradation software)
- Cells, which are basically equilibrium batch reactors that, linked in series, can provide a reasonably accurate description of transport through selected parts of the system (e.g., the engineered barrier system)
- Response surfaces, which take the form of multidimensional tables representing the results of modeling with detailed process models before running the TSPA code (e.g., thermal hydrologic input)
- Functional or stochastic representations of a model component built directly into the GoldSim architecture.

The method used for each TSPA-LA model component is described briefly below.

As in the TSPA-SR, much of the computational work that will go into the TSPA-LA model will be done outside of GoldSim before running the actual total system computations. For example, the UZ flow fields will be computed using TOUGH2 (LBNL 2000 [114091]), a three-dimensional, finite-volume numerical simulator representing the entire UZ model domain (for the dual-permeability model). Other model components that will also be run using computer codes outside of GoldSim include drift-scale thermal hydrology (NUFT (CRWMS M&O 2000 [155731])), in-drift and in-package chemistry (EQ3/6 (CRWMS M&O 1998 [149359])), and SZ radionuclide transport (FEHM). The results of these detailed process-level runs will provide multidimensional tables that will be read into GoldSim at run time. Examples of these multidimensional tables include liquid flux and velocity fields for the UZ and temperature versus time at location within the EBS.

Figure 5.2-2 provides another representation of the TSPA-LA code architecture (i.e., the actual computer codes used and the connections [information transfer] between codes). It includes both the codes run before the GoldSim program and those run in real time that are coupled to (external function calls), or within (cells and tables), the GoldSim program. As shown in Figure 5.2-2, some response surfaces generated by codes external to GoldSim only provide data to other codes external to GoldSim. Other response surfaces, such as liquid saturation, temperature, and seepage flux, will provide data directly into GoldSim as response surfaces that influence such things as waste form degradation rates.

Coupling of the various models will be affected by the climate model, which will impact almost all the other models in one way or another, because it will alter water flow throughout the system. The climate will be assumed to shift in a series of step changes between three different climate states in the first 10,000 years: present-day climate, monsoon climate (about twice the precipitation of the present day climate), and glacial transition climate (colder than monsoon but similar precipitation). These climate shifts will be implemented as a series of steady-state flow fields in the UZ and SZ (including changes in the water table elevation). Within the GoldSim program, these shifts require coordination among the coupled submodels because they must all simultaneously change to the appropriate climate state.

In general terms, the coding methods and couplings to be used for the major components will be similar to those used for the TSPA-SR and are discussed below.

Unsaturated Zone Flow, Mountain Scale-This process will be modeled directly with the three-dimensional, site-scale, UZ flow model using a volume-centered, integral-finite-difference, numerical flow simulator called TOUGH2. Steady-state flow will be assumed, and three-dimensional flow fields will be generated for three different infiltration boundary conditions, three different climate states, and several values of rock properties. These "pregenerated" flow fields (i.e., developed externally and before the GoldSim simulations) will then be placed in a library of files to be read by the finite element heat and mass code (FEHM) for UZ transport during the real time GoldSim simulations. Fracture and matrix liquid fluxes, along with liquid saturation, will be passed to FEHM in these tables. To generate the library of flow fields, an inverse model, ITOUGH2 (Finsterle 1999 [104367]) will be used to calibrate the model-predicted ambient liquid saturations and other properties to measured liquid saturations and other properties in the matrix. This calibration will be done when generating the flow fields for the three different infiltration (developed using INFIL (USGS 2001 [139422])) conditions and the different fracture properties at present-day climate conditions. For future-climate conditions, flow fields will be generated based on the present-day climate calibrations. Climate change will be modeled within TSPA-LA UZ calculations by assuming a series of step changes in boundary conditions, meaning that different flow fields will be provided at the appropriate time with the assumption of instantaneous pressure equilibrium. Based on the particular history of climate changes sampled by the TSPA model at the beginning of a given realization, the UZ flow field library will be interrogated for a different flow field every time during the simulation that a step change is indicated. This change in a flow field will be assumed to apply instantaneously to the transport model. The UZ flow fields will also be provided to the TOUGH2 drift-scale seepage models, to the SZ models, and to the EBS transport models. UZ hydrologic properties are passed to the EBS thermal hydrologic model.

Unsaturated Zone Flow, Seepage of Water into Emplacement Drifts (i.e., Drift Scale)-This process will be also modeled externally before the GoldSim simulations using TOUGH2 on a finely discretized grid around the drift and then abstracted for use in GoldSim. Simulations will be conducted for both ambient and thermal periods over a heterogeneous fracture permeability field for a range of percolation rates (from the mountain scale UZ flow model), and fracture permeability and fracture “alpha” values. These simulations will produce, for both the thermal and ambient periods, two uncertain response surfaces, one for seepage flux into the drift as a function of long-term percolation flux and another for the number of packages that are dripped on (by seeps) as a function of long-term percolation flux. Long-term percolation flux for both ambient and thermal periods is expected to come from the MSTH model at locations sufficiently far above the emplacement drifts to ensure that it is unperturbed by the thermal field.

EBS Environment, Thermal Hydrology-This process will be modeled with the finite-difference computer program NUFT in one, two, and three dimensions before the GoldSim TSPA-LA simulations. Time-dependent thermal-hydrologic variables will be abstracted from these simulations for each of the repository level bins. Abstracted outputs will include:

- Waste package surface temperature and waste package surface RH for seven different package types within discrete environments. These values will be provided to drip shield, waste package, and waste form models in GoldSim.
- Average waste form temperature and liquid saturation in the invert in each of the five repository level bins. Waste form surface temperature will be assumed to be equal to the waste package surface temperature. These temperature and saturation values will be provided to the waste form degradation and EBS transport models in the GoldSim program.
- Average drift wall temperature, RH, evaporation rate, and liquid saturation in the invert in the proposed repository. These values will be provided to the EBS chemical environment models. The outputs will be in the form of response surfaces or multidimensional tables.
- Long-term percolation flux above the drift. These values will be used as inputs to the seepage response surface.

EBS Environment, Drift-Scale Thermal-Hydrologic-Chemical Processes-These processes will be modeled with the computer program TOUGHREACT (LBNL 2001 [153101]) in two-dimensions before the TSPA-LA GoldSim simulations. Simulations will be run for two representative repository locations. Time histories of drift seepage composition and gas composition (representative values for CO_2 and the major aqueous species) will be abstracted from these simulations in tabular form and used as input tables (boundary conditions) for the EBS chemical environment model simulations discussed next.

EBS Environment, Engineered Barrier System Chemical Environment-The chemical environment variables will be modeled with the computer program EQ3/6. Batch-reaction calculations with EQ3/6 will be performed for the boundary condition seepage and gas compositions provided by the drift-scale THC model and a range of representative seepage fluxes and evaporation rates. Output will be response surfaces of various chemical composition parameters. These values will be provided to GoldSim directly as input tables for the waste package/drip shield degradation, invert radionuclide-dissolved concentration, and invert colloid models within GoldSim. The tables provide water composition values for specific input values of carbon dioxide fugacity, temperature, RH, and the ratio of water evaporation flux to incoming water flux.

Waste Package and Drip Shield Degradation-This process will be modeled within GoldSim using the WAPDEG computer code, which includes corrosion-rate variability both on a given package and from package to package. The code will be linked to GoldSim and run at the start of each realization to provide output in the form of several tables of the cumulative number of package failures per time, average patch area per package versus time, average crack area per package versus time, and average pit area per package versus time.

Waste Form Degradation and Mobilization, Cladding Degradation-This process will be modeled within GoldSim using functional relationships that lead to a percentage value of failed cladding versus time. Other cladding degradation modes such as mechanical failure will also be modeled within the GoldSim program. The major inputs to the cladding process model are measured characteristics (examples: oxide thickness, fission gas release) of commercial spent fuel which were collected and fit with first or second order equations. The input parameters for the abstraction will be (1) peak waste package surface temperature, (2) water ingression rate into the waste package, and (3) temperature and chemical composition of the water inside the waste package.

Waste Form Degradation and Mobilization-This process will be modeled by equations within the GoldSim program using empirical degradation rate formulas developed from available data and experiments for the three different waste form types: CSNF, DSNF, and HLW. Output from the waste form degradation model will be the mass of waste form exposed per time and the volume of water in contact with this waste form versus time, which will be used directly in the GoldSim waste form cells. There will be several waste form cells in the GoldSim program, corresponding to different waste form types and seepage cases. The amount of inventory that can ultimately enter each waste form cell will be a linear function of the number of packages emplaced in each inventory, seepage, and thermal hydrologic environment.

Engineered Barrier System Flow and Transport-This process will be modeled directly within GoldSim at run time, using the algorithm embedded in GoldSim cells. The modeling will be based on an idealized representation (basically a linked series of equilibrium batch reactors) of drip shield, waste package, waste form, and invert, and how radionuclides move through them via diffusion and advection both as solutes and as colloids. Output from EBS transport will be radionuclide mass flux (for each of the modeled radionuclides) at each time step, passed during the GoldSim simulations to the directly coupled, three-dimensional, dual-permeability, FEHM particle tracker used for UZ transport. As was implemented in the TSPA-SR, it is expected that the repository area will be divided into five bins based on infiltration; however, this aspect of the model is being evaluated and an alternative approach may be utilized. The mass releases from these five source-term groups will enter the grid blocks in FEHM that reside within the corresponding areas of the regions. The number of grid blocks receiving release will be dependent on the number of packages failed. A key part of EBS transport will be waste form or radionuclide mobilization, which will be a direct function of both seepage flux and radionuclide solubility in the groundwater. Solubility for the various radionuclides will be input directly into the GoldSim program in various forms (e.g., probability density functions, point values, and explicit functions). Several colloid types will also be modeled in the EBS transport component utilizing GoldSim functions.

Unsaturated Zone Transport-This process will be modeled at run time using the directly coupled, three-dimensional, dual-permeability, finite-element code FEHM, which will be accessed as an external function by the GoldSim program. Flow fields and property sets will be accessed directly by FEHM from table files residing in the TSPA-LA Input Database (see Section 6 for a discussion of input controls and the database). The UZ transport model is based on the UZ flow model and will use the same flow fields (generated by the TOUGH2 UZ flow code) and the same climate states. As with UZ flow, a dual-permeability model will be assumed, and transport will be modeled with the FEHM particle tracker in three dimensions. The FEHM particle tracker transports particles on the same dual-permeability TOUGH2 spatial grid as used in the flow model (using the same material properties, infiltration, and liquid saturation). When the climate shifts, a new TOUGH2 flow field will be provided from the run-time file directory, and the particles will be assumed to be instantly traveling with the new velocities. In addition, for multiple-realization runs, a matrix of uncertain UZ transport property values will be created before simulation time by the GoldSim program and then accessed by FEHM during the simulations. The FEHM code will step through the uncertainty matrix row by row, where each row represents one realization of the uncertain UZ transport parameters, including K_ds (K_d is the measure of the partitioning of the mass of a given radionuclide sorbed or residing on the immobile rock phase to the mass dissolved in the aqueous phase) for each radionuclide, matrix diffusion coefficients, dispersivity, and K_c values (K_c is the measure of the partitioning of the mass of a given radionuclide sorbed or residing on colloidal particles to the mass dissolved in the aqueous phase). Output from the FEHM code at each time step will be mass flux from the fractures and matrix at the water table. The location of these output grid points will be a vertical function of the climate state, increasing in elevation for wetter climates. The fracture and matrix mass fluxes from FEHM will be combined appropriately for each of the four SZ capture zones in four GoldSim mixing cells and then fed to the SZ convolution integral SZ_Convolute at each GoldSim time step.

Saturated Zone Flow and Transport-This process will be modeled using two models of SZ flow and transport. The three-dimensional process level model (FEHM) will be used to calculate the transport of individual radionuclides important to dose. A one-dimensional flow tube model implemented in GoldSim will be used to calculate the transport of daughter radionuclides (radionuclides that form by the decay of other radionuclides) of lesser importance. The models will extend from four source regions at the bottom of the repository at the water table to approximately 18-km distance down gradient. The three-dimensional flow and transport simulations will be done outside the GoldSim program for each of the selected radionuclides over the multiple realizations (at least 100) of uncertain SZ model parameters. These uncertain parameters will likely include effective porosity in the alluvium, K_d in the tuff and alluvium, irreversible and reversible colloidal parameters, longitudinal dispersivity, transverse dispersivity, point source location, horizontal anisotropy and fraction of flow path in the alluvium. The horizontal placement of the point source in each of the four source regions varies stochastically from realization to realization, reflecting uncertainty in the location of releasing waste packages and transport pathways in the UZ. Output from the radionuclide transport simulations will be a set of mass breakthrough curves versus time at approximately 18 km from the repository in the predominant direction of groundwater flow for a constant mass release-rate source term. These breakthrough curves will reside in files in the GoldSim run time directory and will be accessed when needed by the SZ_Convolute external function (which convolutes, or integrates, the real source term with the pregenerated unit breakthrough curves) called by the GoldSim program.

Biosphere-Annual dose to the RMEI will be modeled using BDCFs that convert radionuclide concentrations in groundwater (or volcanic ash) to dose. The BDCFs will be developed outside the TSPA model, using a code that will be developed (ERMYN) in accordance with the *Technical Work Plan for Biosphere Modeling and Expert Support* (BSC 2002 [158379]). The factors will then be entered as stochastic elements in the TSPA model. These factors are multiplied by the radionuclide concentrations in the SZ (or by concentrations in volcanic ash) to compute annual doses, which are the end products of the calculations.

Disruptive Events-Igneous (eruptive and intrusive cases) and seismic events are modeled as separate scenario classes. The igneous scenario class includes the igneous intrusion groundwater transport and volcanic eruption modeling cases. The igneous intrusion groundwater transport modeling case is modeled within the TSPA model. This case utilizes many aspects of the nominal scenario and simply overlays an intrusive event, as characterized by its probability and physical properties (e.g., number of waste packages damaged by intrusion, extent of damage to waste packages, etc). After these effects are incorporated to the model, releases are handled as in the nominal scenario. The volcanic eruption case (i.e., radionuclides carried by ash plumes from volcanic eruptions) is modeled using the code ASHPLUME that is directly coupled to the TSPA model at run time. Similar to the igneous intrusion groundwater transport modeling case, the seismic scenario class utilizes many aspects of the nominal scenario and simply overlays a seismic event, as characterized by its probability, level of ground motion or fault displacement (if screened in), and damage to the EBS (e.g., number of waste packages damaged by ground motion, extent of damage to waste packages, etc.).

5.3 IMPLEMENTATION OF SCENARIO CLASSES

5.3.1 Nominal Scenario Class

The nominal scenario class includes all relevant processes that must be integrated to yield an assessment of system performance. Each of the TSPA model components and the flow of information described in Sections 5.1 and 5.2 will be used to evaluate the nominal performance of the proposed repository (see Figure 5-2). The nominal scenario class will incorporate FEPs that are expected to occur throughout the period of interest (i.e., the expected FEPs). The FEPs that have a low (less than 1.0) probability of occurring over the period of interest (i.e., the disruptive FEPs), will be considered in the disruptive event scenario classes that are analyzed both separately and in combination with the nominal case.

5.3.2 Disruptive Event Scenario Classes

Igneous Scenario Class-The two modeling cases considered for TSPA-LA are the volcanic eruption and igneous intrusion groundwater transport modeling cases. They are described in this section.

The volcanic eruption modeling case will consider the direct transport of waste to the ground surface from the repository in a volcanic eruption. This modeling case will begin with an eruptive event, which will be characterized in the TSPA by both its probability and its physical properties such as volume of the eruption, composition of the magma, and properties of the pyroclastic ash. Interactions of the eruption with the proposed repository will be described in terms of the damage to the EBS and the waste package. Characteristics of the waste form in the eruptive environment will be described in terms of waste particle size. Atmospheric transport of waste in the volcanic ash plume begins with entrainment of waste particles in the pyroclastic eruption and will be affected by wind speed and direction. BDCFs will be developed for exposure pathways relevant to atmospheric deposition of contaminated ash with detailed attention to important pathways, rather than for the groundwater pathways considered for nominal performance. As a final step, the volcanic eruption BDCFs will be used to determine radiation doses resulting from exposure to contaminated volcanic ash at approximately 18 km from the proposed repository in the predominant direction of groundwater flow.

Implementation of the volcanic eruption event in TSPA-LA is illustrated in Figure 5.3-1. Information about eruption characteristics, the probability of eruptive conduits forming within the proposed repository, and the proposed repository response to eruption will be used to develop a distribution of parameter values characterizing uncertainty in the extent of damage to waste packages and the amount of waste available to be entrained in the eruption. Entrainment of waste and atmospheric transport of contaminated ash will be modeled using ASHPLUME, yielding a distribution of results characterizing uncertainty in the concentration of waste particles on the ground surface. BDCFs calculated for the volcanic eruption modeling case will be used to calculate doses.

The igneous intrusion groundwater transport modeling case will consider an igneous intrusion that travels down the drifts and remains underground. Although the intrusion damages waste packages and other components of the EBS, FEPs analyses have concluded that it does not significantly alter the long-term flow of water through the mountain (CRWMS M&O 2000 [151553], Section 6.2.16). As shown in Figure 5.3-2, the igneous intrusion groundwater transport model will use information about the probability of intrusion, the characteristics of the intrusion, and the response of the proposed repository to calculate damage to waste packages. Groundwater transport away from the damaged packages will be calculated using the nominal scenario class models, and doses to humans from contaminated groundwater are determined using nominal BDCFs.

As in the TSPA-SR, the probability of future igneous activity in the Yucca Mountain region that will be used in the TSPA-LA is based on the *Probabilistic Volcanic Hazard Analysis for Yucca Mountain, Nevada* (CRWMS M&O 1996 [100116]) conducted in 1995 and 1996. Ten experts in the field of volcanology evaluated available data on past volcanic activity in the region and provided expert judgment on the probability of future igneous activity. Their judgments (elicitations) were then combined to produce an integrated assessment of the volcanic hazard that reflects a range of alternative scientific interpretations. Details of the identification of the experts, presentation of available data to them, and the elicitation process are available in the summary report of the probabilistic volcanic hazard analysis (CRWMS M&O 1996 [100116]).

Specific information developed to support the TSPA-LA models for igneous disruption of the proposed repository includes the following:

- The geometry of an intrusion: dike width, length in the proposed repository, azimuth, and the number of dikes that could occur as part of a single intrusive event.
- The geometry of an eruption: conduit diameter at the proposed repository depth, and the number of conduits (also called eruptive centers and vents) that intersect drifts and that could be associated with a single intrusive event.
- Physical and chemical properties of the magma: temperature, density, volatile content.
- Intrusive properties: magmatic ascent velocity, magmatic phase changes as drifts are encountered.
- Eruptive properties: pyroclastic ascent velocity, eruption power, eruption duration, eruption volume (mass discharge rate), ash particle size and shape, ash density.
- Dike and proposed repository interactions: environmental conditions in the drift, response of the waste package, extent of the magmatic damage in the drifts (including the number of waste packages damaged by both intrusion and eruption), behavior of the waste form in the eruptive environment.
- Atmospheric properties: wind speed and direction, ash dispersion, air density and viscosity.

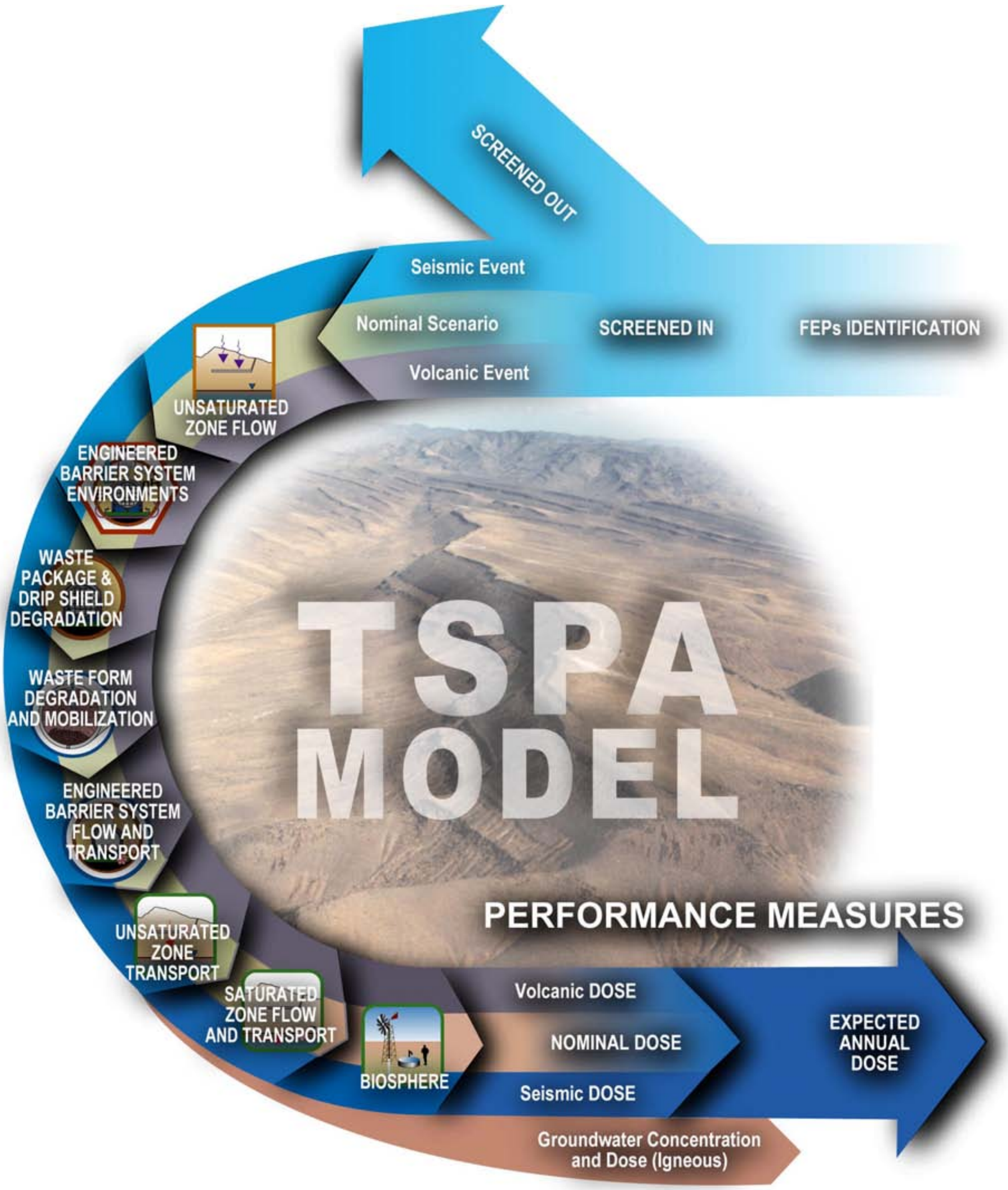
Seismic Scenario Class-The seismic scenario class considers the potential effects from an earthquake that occurs near the repository. Although the subsequent ground motion and potential fault displacement at the repository horizon may damage waste packages and other components of the EBS, FEPs analyses indicate that these seismic hazards will not significantly alter the long-term flow of water through the mountain. This will be documented in a FEPs AMR. As shown in Figure 5.3-3, this scenario class begins with a seismic event. Seismic waves subsequently propagate to the repository causing ground motion at the repository horizon, which will be characterized in the TSPA-LA by its probability and amplitude. Fault displacement may also occur. These seismic hazards may cause damage to drip shields, waste packages, and cladding. Radionuclides are then released from damaged waste packages and subsequently transported by the groundwater to the biosphere. Groundwater transport away from the damaged packages will be calculated using the nominal scenario class models, and doses to humans from contaminated groundwater are determined using nominal BDCFs.

Specific information developed to support the TSPA-LA model for seismic damage to the proposed repository will include the following:

- The annual frequency of occurrence for mean ground motion events and the mean fault displacement hazard curves. This information has been documented in the probabilistic seismic hazard analysis (PSHA) report (CRWMS M&O 1998 [103731]).

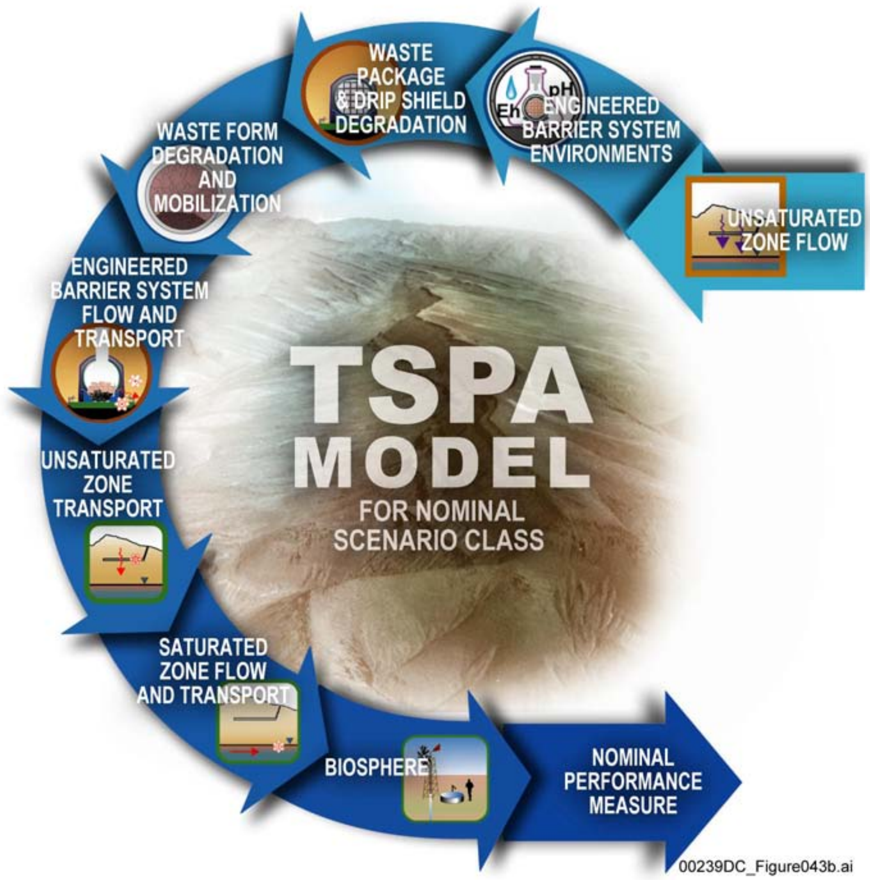
- Ground motion seismic design inputs, which will be determined from: (1) the PSHA analysis for Yucca Mountain, and (2) a ground motion model for specific locations at the site. The PSHA analysis determines ground motions for a hypothetical site that has the dynamic characteristics of rock found at a depth of 300 meters beneath Yucca Mountain. The ground motion model for specific locations at the site starts with the results of the PSHA analysis for a particular annual mean frequency of exceedance and determines the ground motion at depth by including the effect(s) of the overlying rock and/or soil on ground motions. Fault displacement design inputs will be determined from the PSHA analysis for Yucca Mountain and the site-specific fault displacement hazard curves at the emplacement drifts.
- The response of the waste package, drip shield, and cladding as a function of levels of ground motion, rockfall, and fault displacement for degraded component states that correspond to the 10,000 year compliance period. Detailed structural response calculations will be performed for the drip shield and waste package under loads from rockfall and vibratory ground motion. A more simplified approach may be used for cladding, based on a fragility curve that quantifies the conditional probability of cladding failure.
- Damage from seismic events will be represented as a failed area on the surfaces of the drip shield and waste package, and as a failed cladding area on the fuel rods. These failed areas allow flow through the drip shield and transport from the waste package. This release mechanism (via a failed area) is similar to the nominal scenario class, although the processes generating the failed areas are different. For the nominal scenario class, general corrosion generates failed patch areas on the waste package and drip shield and localized corrosion generates stress corrosion cracks on the waste package. For the seismic scenario class, structural response to rockfall and vibratory ground motion may result in structural deformation and residual stress that leads to failed areas from accelerated stress corrosion cracking. In either class, the presence of failed areas provides the potential for diffusive and advective transport out of the waste package, through the EBS, and into the unsaturated zone.

In summary, the TSPA-LA model for the seismic scenario class is very similar to the TSPA-LA model for the nominal scenario class, with two major exceptions: (1) the failed area for the drip shield or waste package is determined by sampling a failed area response curve, rather than by calculations with WAPDEG for expected degradation and corrosion processes; and (2) a single seismic event sufficient to induce degradation of the engineered barriers occurs at a random time during each realization.



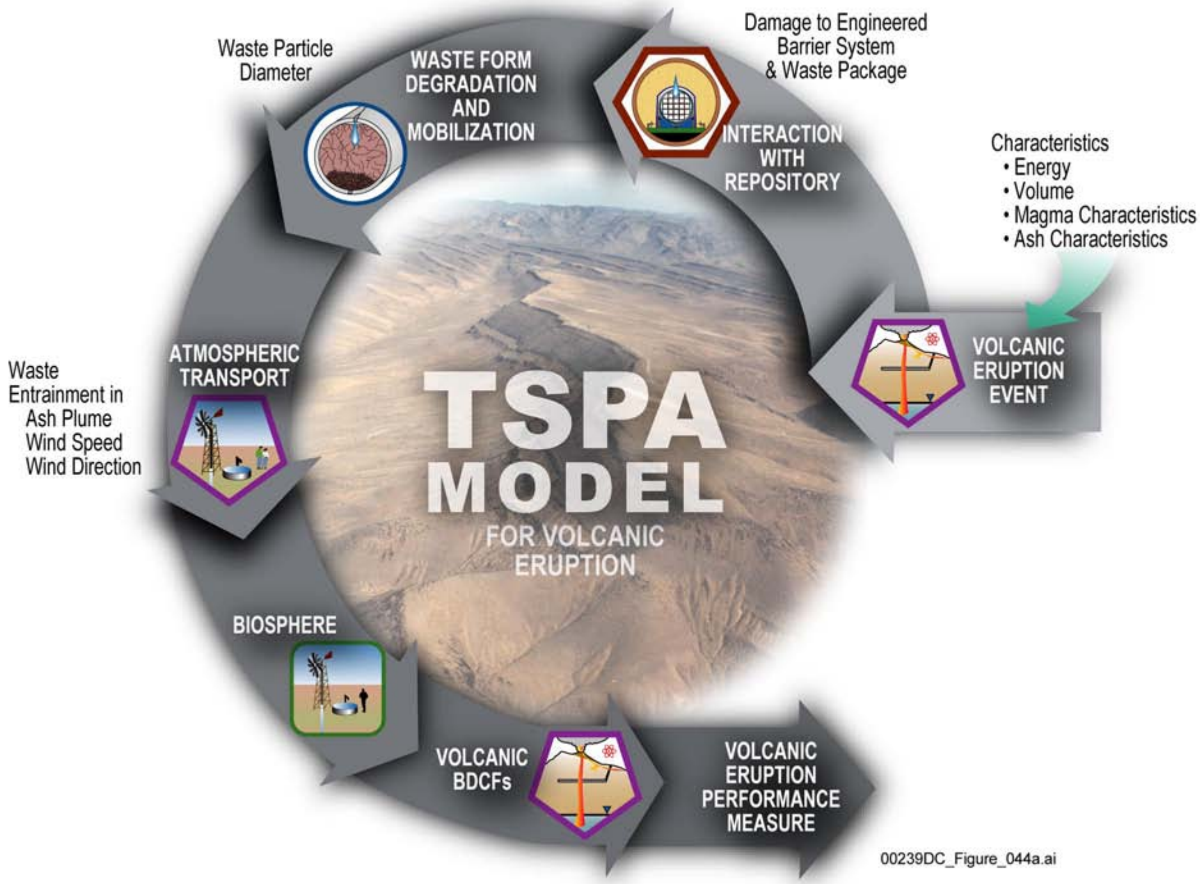
Source: Modified from CRWMS M&O 2000 [153246], Figure 2.1-5.

Figure 5-1. Schematic Representation of the Development of Total System Performance Assessment-License Application Including the Nominal, Igneous, and Seismic Scenario Classes



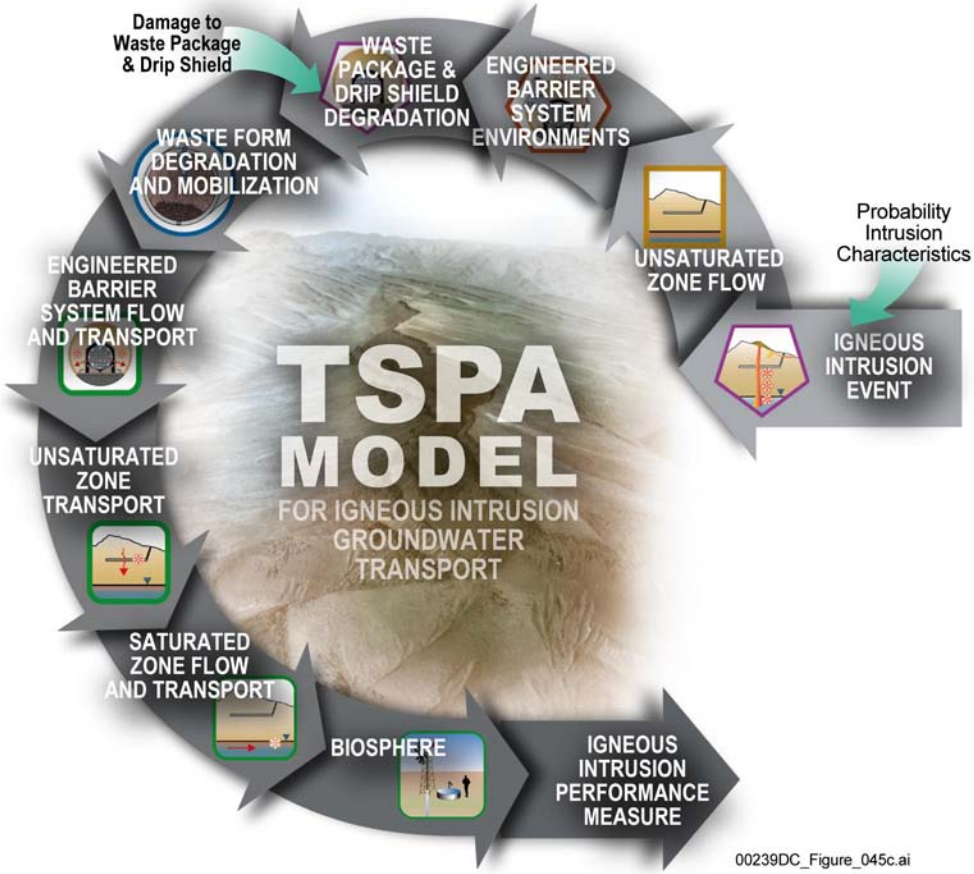
Source: Modified from CRWMS M&O 2000 [153246], Figure 2.1-6.

Figure 5-2. Schematic Representation of the Model Components of the Total System Performance Assessment-License Application Nominal Scenario Class



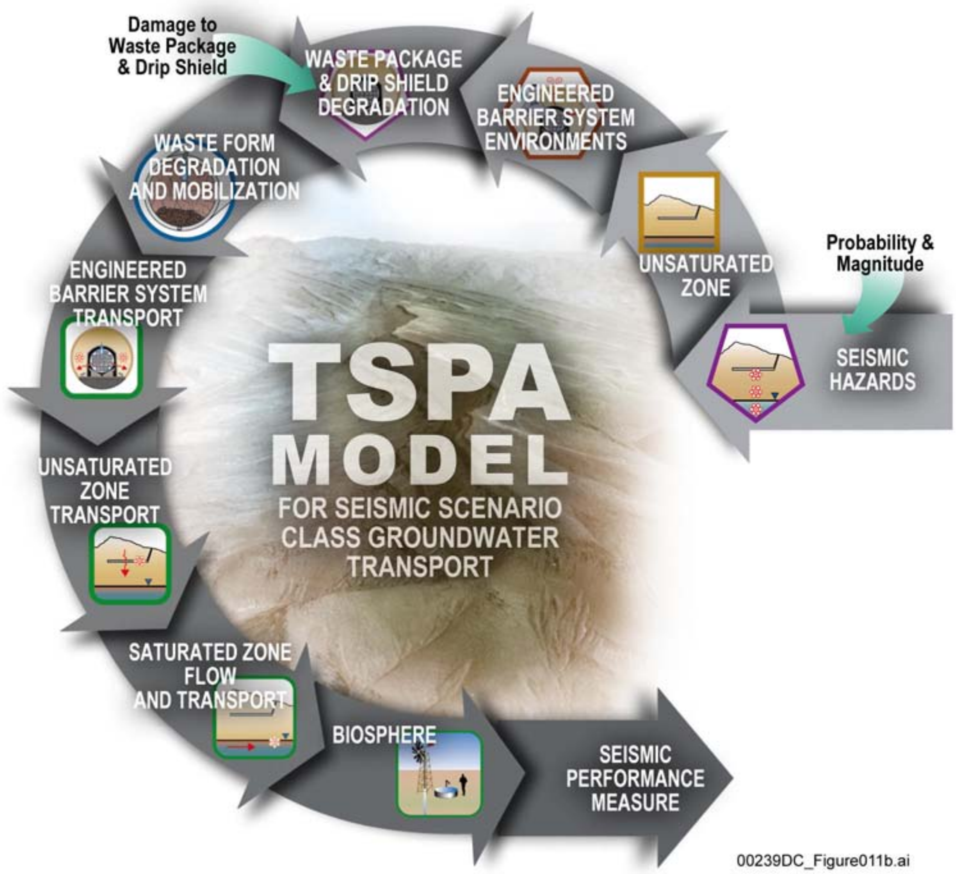
Source: Modified from CRWMS M&O 2000 [153246], Figure 3.10-2.

Figure 5-3. Schematic Representation of the Total System Performance Assessment-License Application Model Components of the Volcanic Eruption Modeling Case



Source: Modified from CRWMS M&O 2000 [153246], Figure 3.10-3.

Figure 5-4. Schematic Representation of the Total System Performance Assessment-License Application Model Components of the Igneous Intrusion Groundwater Transport Modeling Case



Source: Modified CRWMS M&O 2000 [153246], Figure 3.10-3.

Figure 5-5. Schematic Representation of the Total System Performance Assessment-License Application Model Components of the Seismic Scenario Class

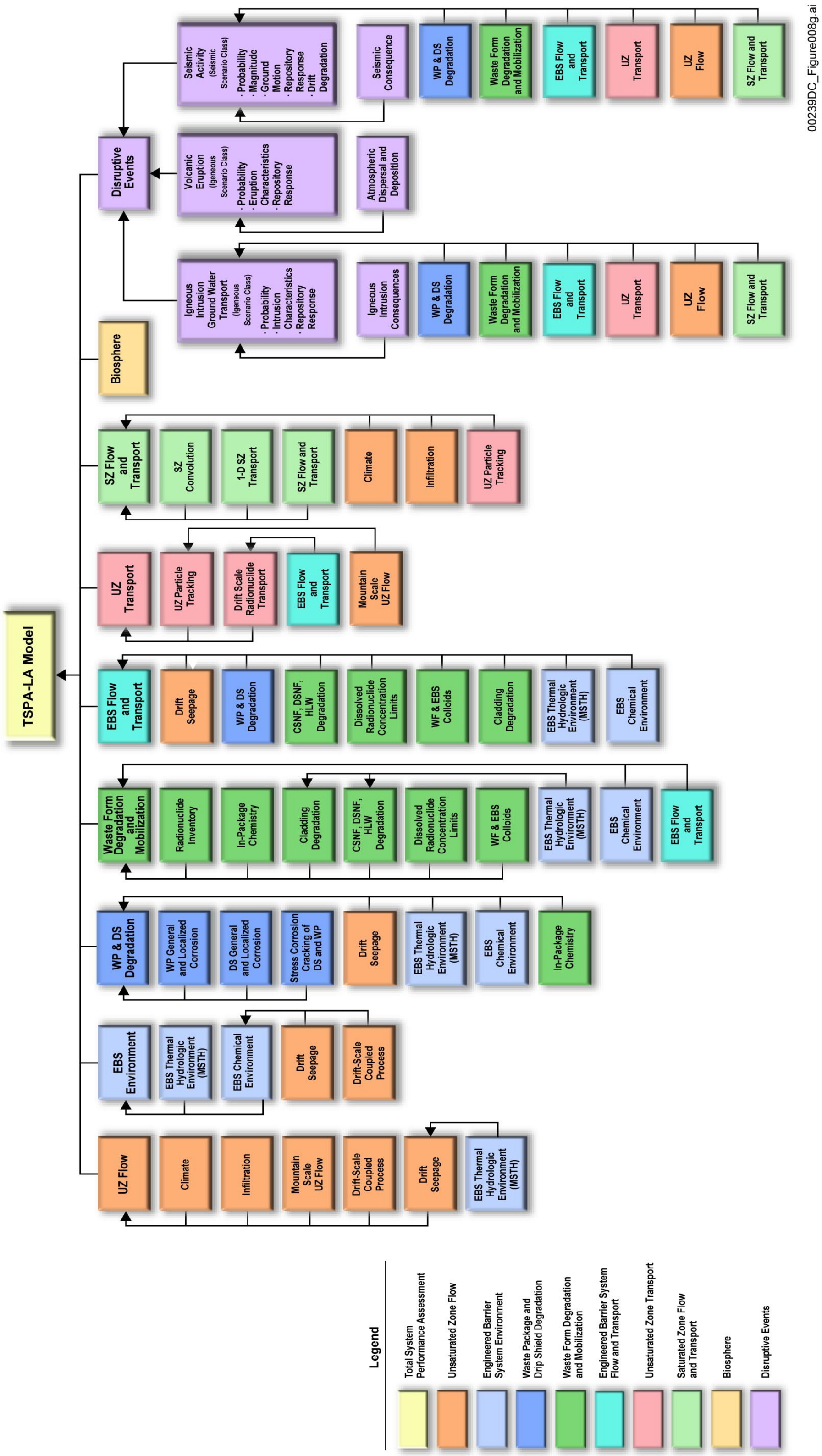
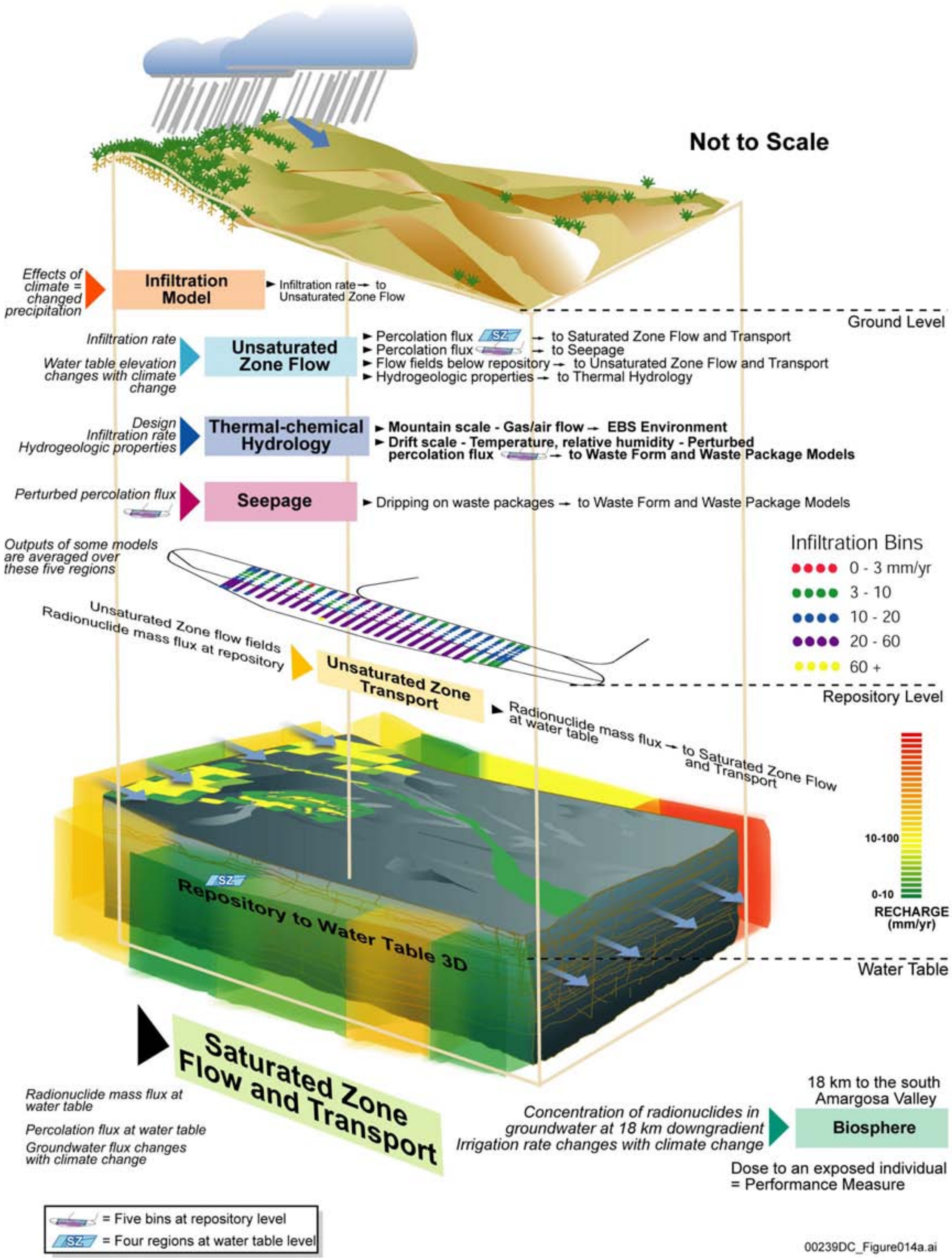


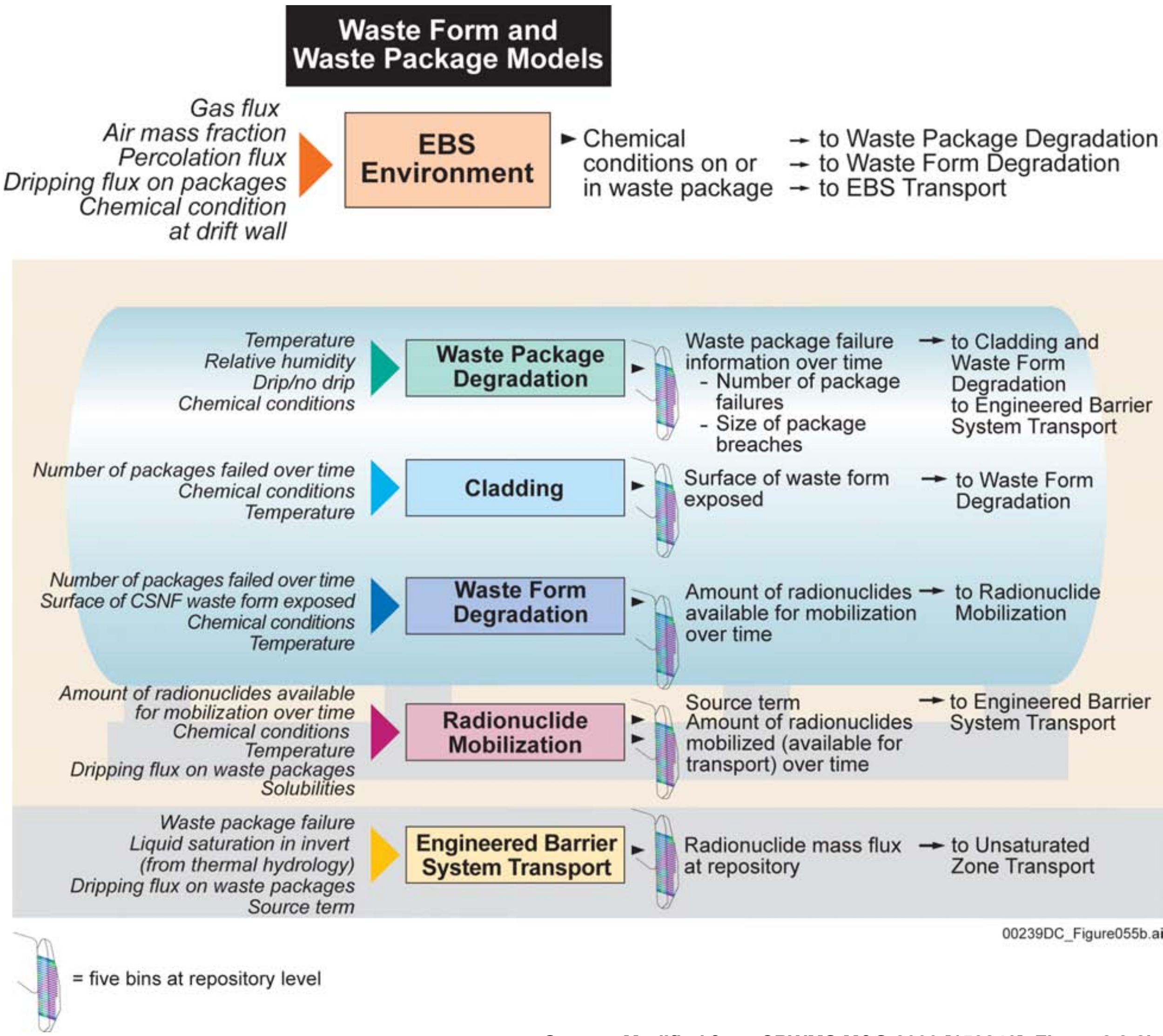
Figure 5.1-1. Total System Performance Assessment-License Application Model Components and Submodels



Source: Modified from CRWMS M&O 2000 [153246], Figure 2.2-2a.

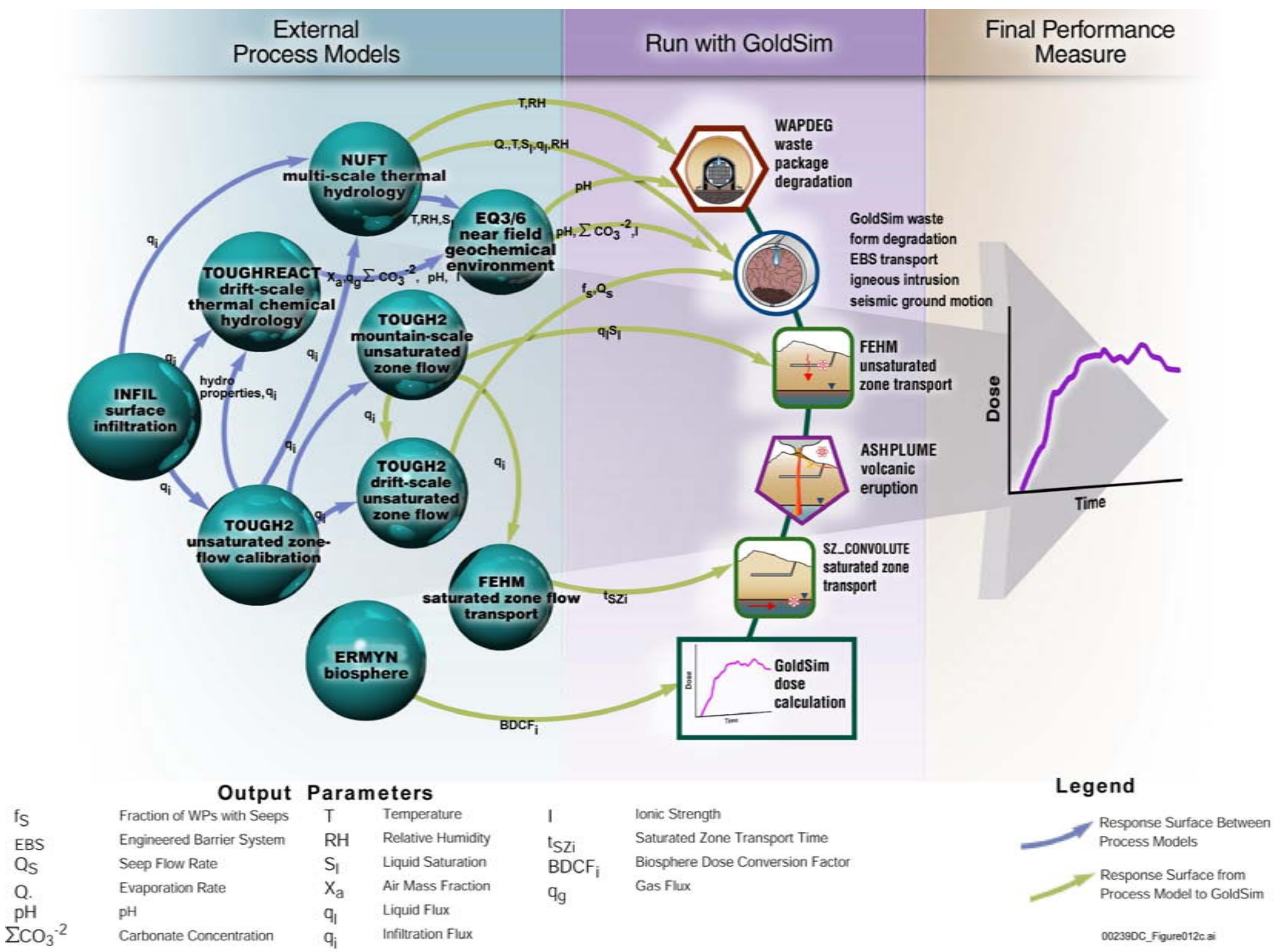
NOTE: The Figure is in two parts with the detail of the waste package and waste form models shown in Figure 5.2-1b.

Figure 5.2-1a. Detailed Representation of Planned Information Flow in the Total System Performance Assessment-License Application



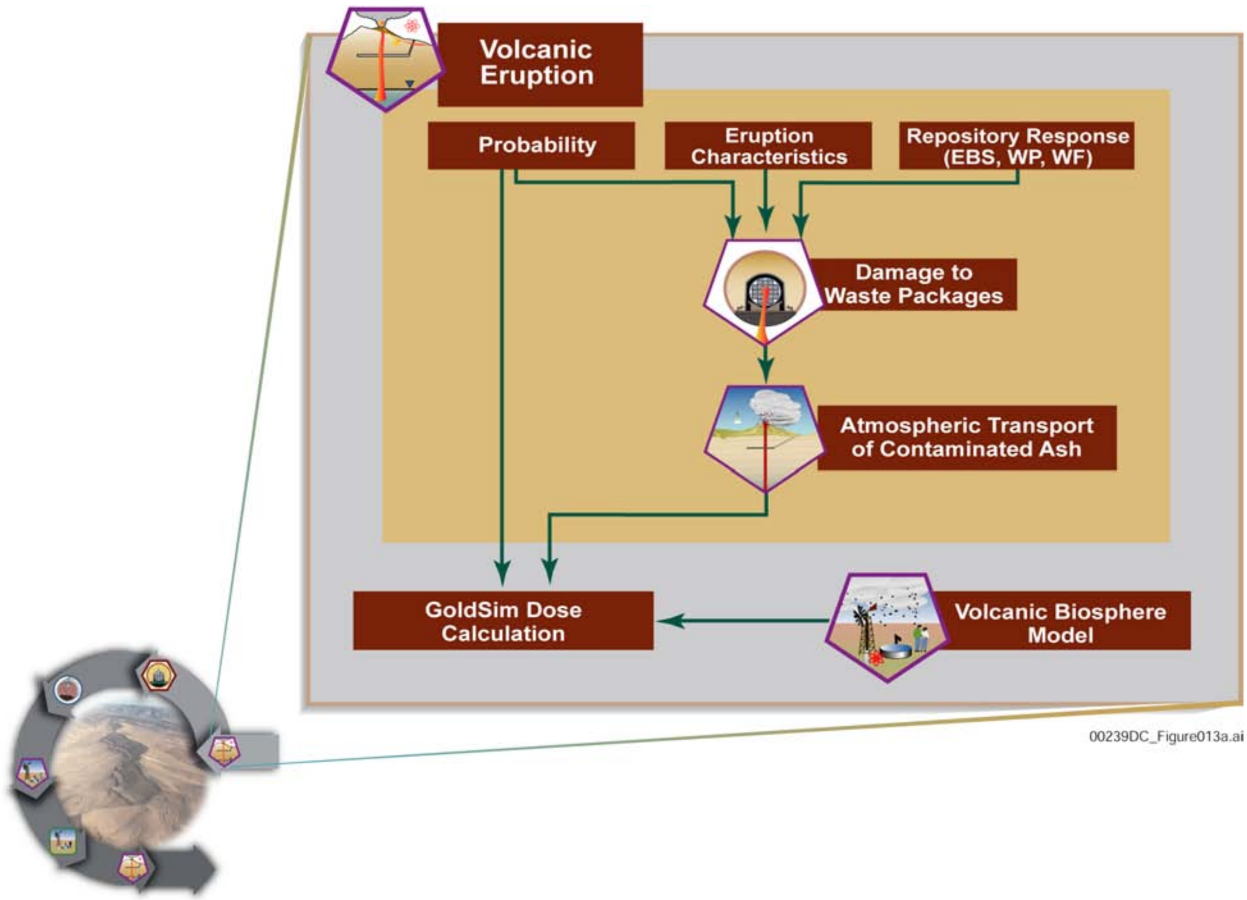
Source: Modified from CRWMS M&O 2000 [153246], Figure 2.2-2b.

Figure 5.2-1b. Detailed Representation of Planned Information Flow in the Total System Performance Assessment-License Application



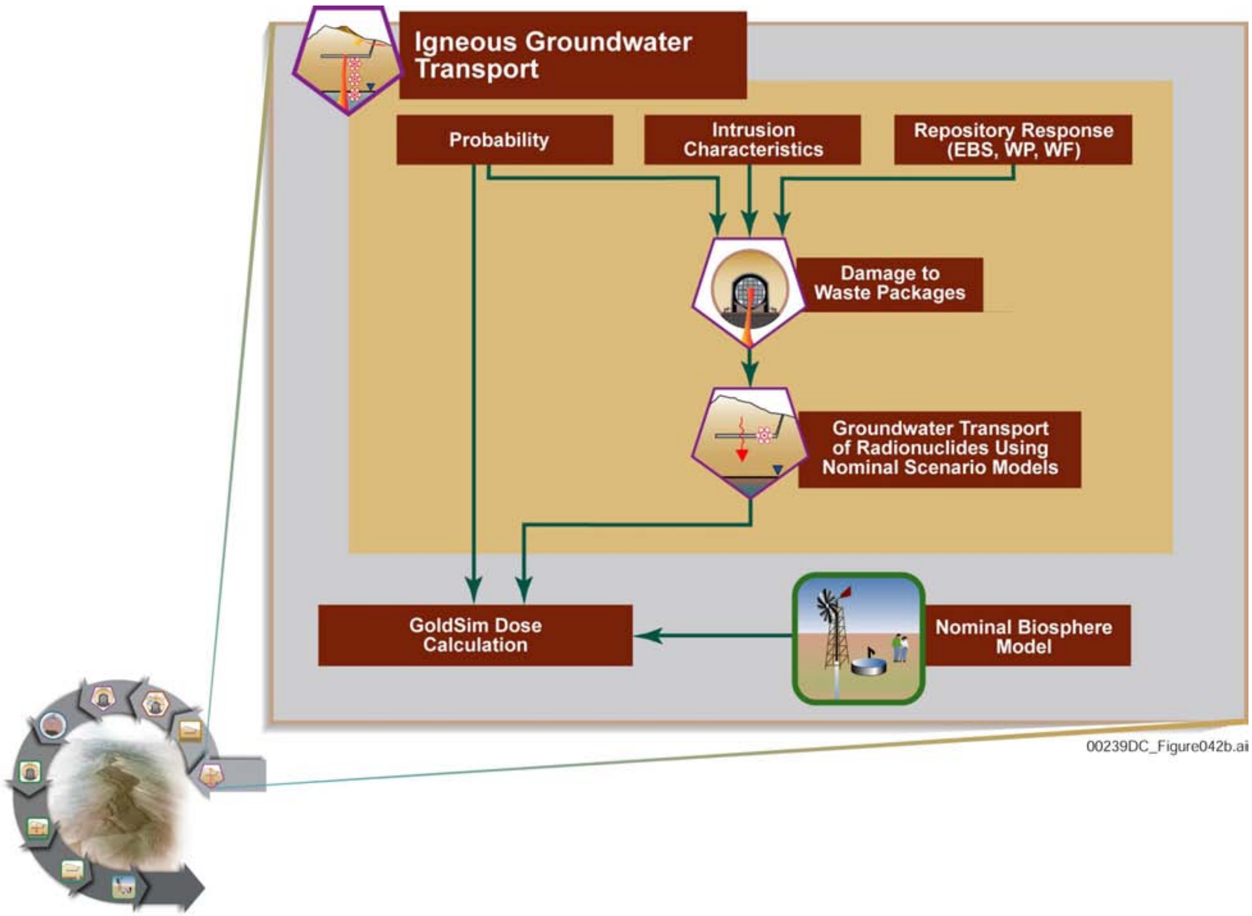
Source: Modified from CRWMS M&O 2000 [153246], Figure 2.2-3.

Figure 5.2-2. Total System Performance Assessment-License Application Code Configuration: Information Flow Among Component Computer Codes



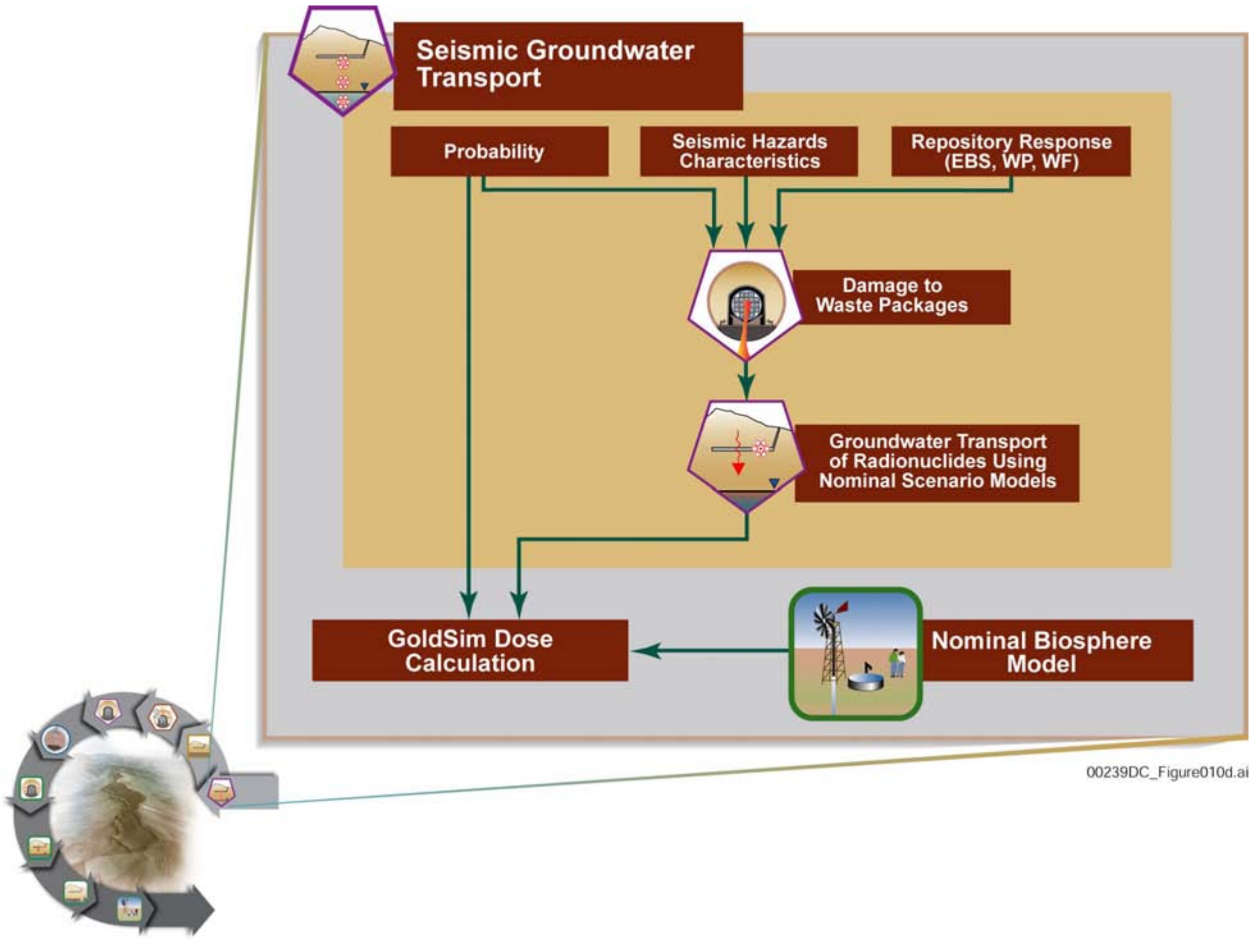
Source: CRWMS M&O 2000 [153246], Figure 3.10-6

Figure 5.3-1. Information Flow within the Volcanic Eruption Model



Source: CRWMS M&O 2000 [153246], Figure 3.10-11.

Figure 5.3-2. Information Flow within the Igneous Intrusion Groundwater Transport Model



Source: Modified from CRWMS M&O 2000 [153246], Figure 3.10-11.

Figure 5.3-3. Information Flow within the Seismic Groundwater Transport Model

6. CONTROL OF THE TSPA-LA MODEL

This section discusses control of the TSPA-LA model. The controls are applicable for model development, model testing, correction of model errors, and the production of TSPA simulations (including the compliance simulations for the License Application). The controls cover the entire life-cycle of the model, from management direction of what changes are to be made to the model, to the control of completed TSPA simulations and their results. It should be noted that these controls do not replace the QA procedures that govern work involving the TSPA-LA model, rather they provide additional guidance for implementing the requirements of the QA procedures. The controls and guidelines for this work will be documented in a controlled document for use by all TSPA analysts (*Total System Performance Assessment Model Desktop Guidelines*, currently in draft). All documentation generated in the control processes will be filed in the records system with the TSPA-LA documentation.

6.1 DESCRIPTION OF THE TSPA MODEL

The TSPA-LA model consists of four major parts, the GoldSim model file, the DLLs called by the GoldSim model file, the set of input files used by DLLs, and the database which passes input parameters to the GoldSim model file.

There is also a three-tier hierarchy of analysis cases for the TSPA-LA model: the master case, base cases, and sensitivity cases (see Figure 6.1-1). The master case is designed to simulate multiple performance assessment scenario classes. A base case is produced when the master case is run for a given scenario class case and set of simulation settings (e.g. nominal scenario class, 300 realizations, 20,000-year duration). A sensitivity case is produced when a base case is run with a change to the model (e.g., neutralization of drip shield sensitivity case).

6.2 MANAGEMENT CONTROL

The TSPA-LA model may require modification for a number of reasons. The management control of these changes is presented in this section, and illustrated in Figure 6.2-1.

New or revised AMRs being developed for the LA will utilize the FTL/ATL/PTL processes as described in Section 3. During the development of new or revised AMRs, TSPA analysts will be involved with the SMEs in defining the technical output of their AMRs for use in the TSPA-LA model. Draft information (e.g., DTNs and AMRs) will be provided for initial implementation into the TSPA-LA model. The results of the initial implementations will be reviewed by the appropriate SMEs to ensure that the implementation is consistent with the SMEs intent for the model. Any discrepancies will be addressed by changing the implementation in the TSPA-LA model and/or changing the supporting AMRs and/or DTNs prior to their being finalized.

In addition, new or revised AMRs developed for the LA will be reviewed by the TSPA Department as part of the AP-2.14Q, *Review of Technical Products and Data*, of the AMRs. Part of this review will determine whether changes to the TSPA-LA model are required and if they are within the TSPA model development scope and schedule.

Potential changes to the TSPA-LA model due to identified errors will be reviewed by the TSPA Department as part of the disposition of Technical Error Reports (TERs) per AP-15.3Q, *Control of Technical Product Errors*.

Internal TSPA-LA model changes (e.g., change in model logic to set scenario-case specific parameters) will be identified as part of TSPA-LA model development. Changes within the TSPA-LA model development scope and schedule will be approved by the TSPA Department Manager. If the changes are outside the TSPA-LA model development scope and schedule the TSPA Department Manager will elevate the issue to the Performance Assessment Strategy and Scope Manager for resolution. Management approval of changes to the TSPA-LA model will also be predicated on whether the change is necessary to comply with regulatory requirements, if final input feed date has passed for the requested change, or if the TSPA-LA model itself has been finalized or “frozen” for TSPA-LA.

Changes to the TSPA-LA model will be tracked by the TSPA Department. An example form that may be utilized to track the changes is shown in Figure 6.2-2. A similar form is included in the previously mentioned controls and guidance document under development. When the model is in the development stage, written approval from the TSPA Department Manager, TSPA Model Calculations Lead, and TSPA Configuration Management Lead is required for TSPA analysts to change/introduce new process models, model abstractions, or parameters into the TSPA-LA model. The written authorization will specify the source(s) (e.g., AMRs, DTNs, etc.) from which process models, model abstractions, or input parameters are to be taken. If only draft source(s) are available, this will be noted in the authorization.

Changes to TSPA-LA model for the purpose of performing sensitivity studies or other analyses of the TSPA-LA model also require written approval from the TSPA Department Manager, TSPA Model Calculations Lead, and TSPA Configuration Management Lead.

Another important aspect of the control of the TSPA-LA model is to ensure consistent, well-documented inputs. The supporting organizations provide abstractions, and technical product output to the TSPA-LA model. What this content is expected to be was initially determined in a scope and schedule review conducted in early 2002. The scope and schedule reviews were lead by the Performance Assessment Scope and Strategy Subproject and resulted in addition of detail to the Technical Work Plans for each Work Package containing an AMR. The detail was incorporated into revisions to the Technical Work Plans, which specified content for FEPs, ACMs, parameters and uncertainty to be supplied to the TSPA-LA model.

The detailed plan for the systematic treatment of uncertainty in support of the LA products is intimately linked to this overall strategy of placing more management emphasis and control on the development of inputs to the TSPA-LA and the LA itself. These additional product management emphasis and controls include:

- A consistent model hierarchy and structure that feeds the TSPA-LA model architecture
- A consistent treatment and documentation of model abstractions that support the TSPA-LA
- A consistent treatment and documentation of ACMs
- A consistent treatment and documentation of FEPs that are included in the TSPA-LA as well as how they have been included and where their inclusion has been documented
- A consistent evaluation of the definition and performance of the barriers and the basis for the projection of barrier performance
- A consistent evaluation of parameter uncertainty and how that uncertainty is propagated through the model hierarchy to TSPA-LA and how the significance of that uncertainty is evaluated
- A consistent documentation of how the models are integrated and information flows between the models and analyses, including roadmaps of information supporting the TSPA-LA
- A consistent basis for determining the appropriate amount of confidence required for model validation
- A consistent evaluation of what data were used to develop parameter distributions and why those data are sufficient to capture the range of possible observations.

The above emphasis determines much of the content of the AMRs that will support the TSPA-LA and the postclosure safety case to be presented in the License Application. These AMRs remain the primary supporting documentation of the TSPA-LA and the License Application Safety Case as they were in the Site Recommendation document hierarchy. Appropriately assigning this scope, FEP by FEP, model by model, and parameter by parameter into the AMRs has been accomplished in updated Technical Work Plans for each of the supporting AMRs.

The more detailed scope definitions that result from the above process yield a much more consistent and comprehensive treatment of not only parameter uncertainty but also FEP uncertainty and ACM uncertainty. It also allows for early definition of the scope and content of the TSPA-LA within the context of the *TSPA-LA Method and Approach* document as agreed to in several TSPAI KTI agreements. Finally, this more detailed scope definition will allow the AMR authors to focus on the key performance-related aspects of their models and analyses in a more risk-informed way.

6.3 PHYSICAL CONTROL OF FILES

The TSPA-LA model file and its associated input files, DLLs, and database are controlled by storing them in a set of controlled subdirectories on the TSPA file server. Read access to these subdirectories is limited to TSPA Department staff. Write access is limited to the TSPA Model Calculations Lead, the TSPA-LA Configuration Management Lead, and the System Administrator.

Input files for the TSPA-LA model will be obtained from TDMS and stored in a controlled subdirectory on the TSPA file server. A baseline list of files is established by the TSPA-LA Configuration Management Lead. Any subsequent changes to the input files are documented as changes to the baseline list and are initialed and dated by the TSPA Model Calculations Lead and the TSPA-LA Configuration Management Lead.

DLLs for the TSPA-LA model are obtained from SCM, and are installed in a controlled subdirectory on the TSPA file server by the TSPA-LA Configuration Management Lead. A baseline list of DLLs is established by the TSPA-LA Configuration Management Lead. Any subsequent changes to the DLLs are documented as changes to the baseline list and are initialed and dated by the TSPA Model Calculations Lead and the TSPA-LA Configuration Management Lead.

Input parameters (both certain and uncertain) for the TSPA-LA model are controlled by the TSPA Inputs Database. The database is stored in a controlled subdirectory on the TSPA file server.

Completed TSPA-LA model cases are stored in a controlled subdirectory on the TSPA file server. Also, any post-processed results, plots, additional calculations or documentation to support a given case or set of cases will be stored in a controlled subdirectory on the TSPA file server.

6.4 CHANGE CONTROL AND CHECKING

Approved changes to the TSPA-LA model are documented in a conceptual description of the changes, a checklist of the changes to the model, and a change log generated by the GoldSim code. The conceptual description provides an overview of the changes that are to be incorporated into the model. It also contains documentation of any development and testing work that was performed to support the change to the TSPA-LA model. The checklist documents the specific changes made to the model. The change log provides a record of what changes were actually made to the GoldSim model file. The conceptual description, checklist, change log, and TSPA-LA model file are all checked to verify that the changes are correctly implemented into the TSPA-LA model.

A change to TSPA inputs is also documented in the TSPA Inputs Database.

Checking is performed by a qualified individual (assigned by the TSPA Model Calculations Lead), usually another TSPA analyst, who was not involved in modifying the controlled model file or input file(s).

Two types of checks are done on a model; parameter-level checking and conceptual model checking. Parameter-level checking verifies that all of the changes to the model file and/or external files were done correctly. Conceptual model checking considers whether the implementation in the model correctly reproduces the conceptual model (process model or model abstraction) in the associated AMR, model, or scientific analysis.

Parameter-level checking will be documented in a checklist similar to Figure 6.4-1. The steps involved in this check include:

- Check changed/added GoldSim elements against their source information to verify that they were changed correctly.
- Verify that the input links of added elements are correct.
- Verify that the output links of added parameters are correct.
- Check that the links to and from any deleted elements have been appropriately reconnected.
- Verify (by inspecting source references for changes) that each change to an external file is correct.
- A full multiple-realization run of the model will be performed. The results of this run will be evaluated to verify that the correct changes were made to the model.

The conceptual check considers whether the changes to the model correctly reflect the conceptual model changes. The conceptual description should include a general description of the changes made to the model. Any development and testing work to support the changes should also be documented in the conceptual description. General questions that the conceptual check should answer (if applicable, if not applicable then so note) include:

- Does the modified portion of the model respond appropriately to its inputs?
- Do the model components downstream from the modifications respond appropriately?
- Are model inputs and outputs within their specified ranges?
- Can the final dose results be explained in terms of upstream parameters (e.g., waste package/drip shield failure curves, seepage flow, pH, solubilities, EBS release rates)?
- Did the modification(s) invalidate an upstream or downstream conceptual model?
- Is mass conserved within each major subsystem?
- Is energy conserved within each major subsystem?
- Can each entry in the GoldSim run log be shown to have no/negligible impact on the run?
- Is the model implemented correctly for each scenario class?

Any differences between the results of the initial and modified case should be explained and properly documented by the checker in terms of the changes made to the model.

If preliminary AMRs and DTNs are initially used to implement a LA process model/abstracting into the TSPA-LA model, an additional back-check will be made to ensure that the TSPA implementation is consistent with the final AMRs and DTNs.

6.5 MANAGING TSPA-LA MODEL INPUTS (TSPA INPUT DATABASE)

TSPA-LA model input parameters (excluding simulation settings and TSPA system parameters) will be managed by the TSPA Input Database. The database will be developed in Microsoft-Access. The database will not perform any calculations or logical evaluations, rather it strictly acts as a central storage location from which input parameters are downloaded into the GoldSim TSPA-LA model file.

Input parameters will be manually extracted from DTNs stored in the TDMS. The parameter entry forms in a DTN will be used to locate the parameters in the DTN. Input parameters which are accepted data (e.g., atomic weights, radionuclide half-lives, etc.) will be manually extracted from a controlled source. Parameters entered into the database will be checked and verified against their source.

Since the TSPA Input Database is part of the overall TSPA-LA model, it will be developed, controlled, and documented in the same manner as the other parts of the TSPA-LA model.

Figure 6.5-1 illustrates the information flow between TDMS, the TSPA file server, and the TSPA Input Database.

A set of input parameter tables based on the database inputs will be developed as part of the TSPA-LA Model Document. Appendix F contains an example table which illustrates the information to be captured.

6.6 CONTROL OF TSPA-LA MODEL RESULTS

TSPA-LA model results consist of the completed TSPA model simulation files (i.e., cases), information extracted from the model (e.g., plots, tables), and post-processed information.

The TSPA-LA model simulations are documented in a readme file that is submitted as part of the DTN for the simulations. The readme file contains descriptions of the simulations, the supporting documentation, the input files and input parameters, and the software used. A flow chart is also provided (either in the readme file or as a separate file in the DTN submission) which illustrates the relationship between the TSPA-LA master case, the TSPA-LA base cases, and the TSPA-LA sensitivity cases.

Plots of TSPA-LA model results will be documented with a checklist (format will be identified in the aforementioned Controls and Guidelines Document under development within the TSPA Department). The TSPA-LA model cases and the model elements from which results are extracted are documented in the checklist. Additional information such as axis labels, time-scales, data-set labels, etc. will also be verified via the checklist (see Figure 6.6-1 for example checklist).

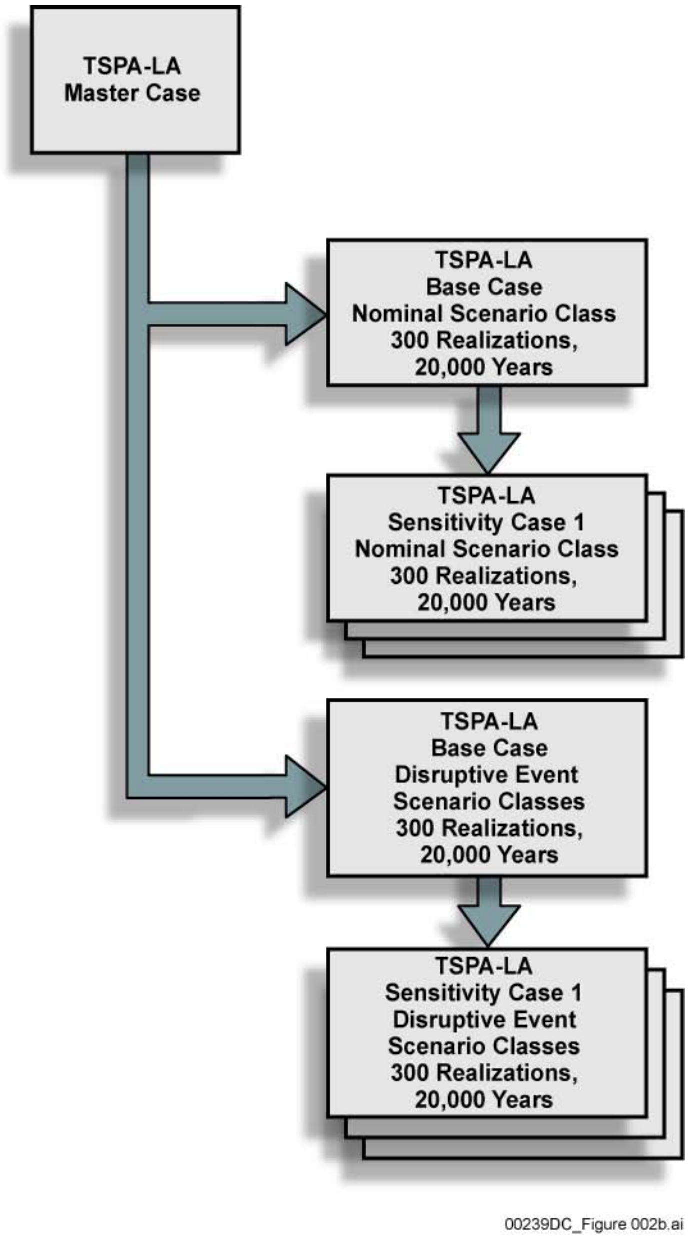


Figure 6.1-1. Example of the Relationship among the TSPA-LA Master Case, Base Cases, and Sensitivity Cases

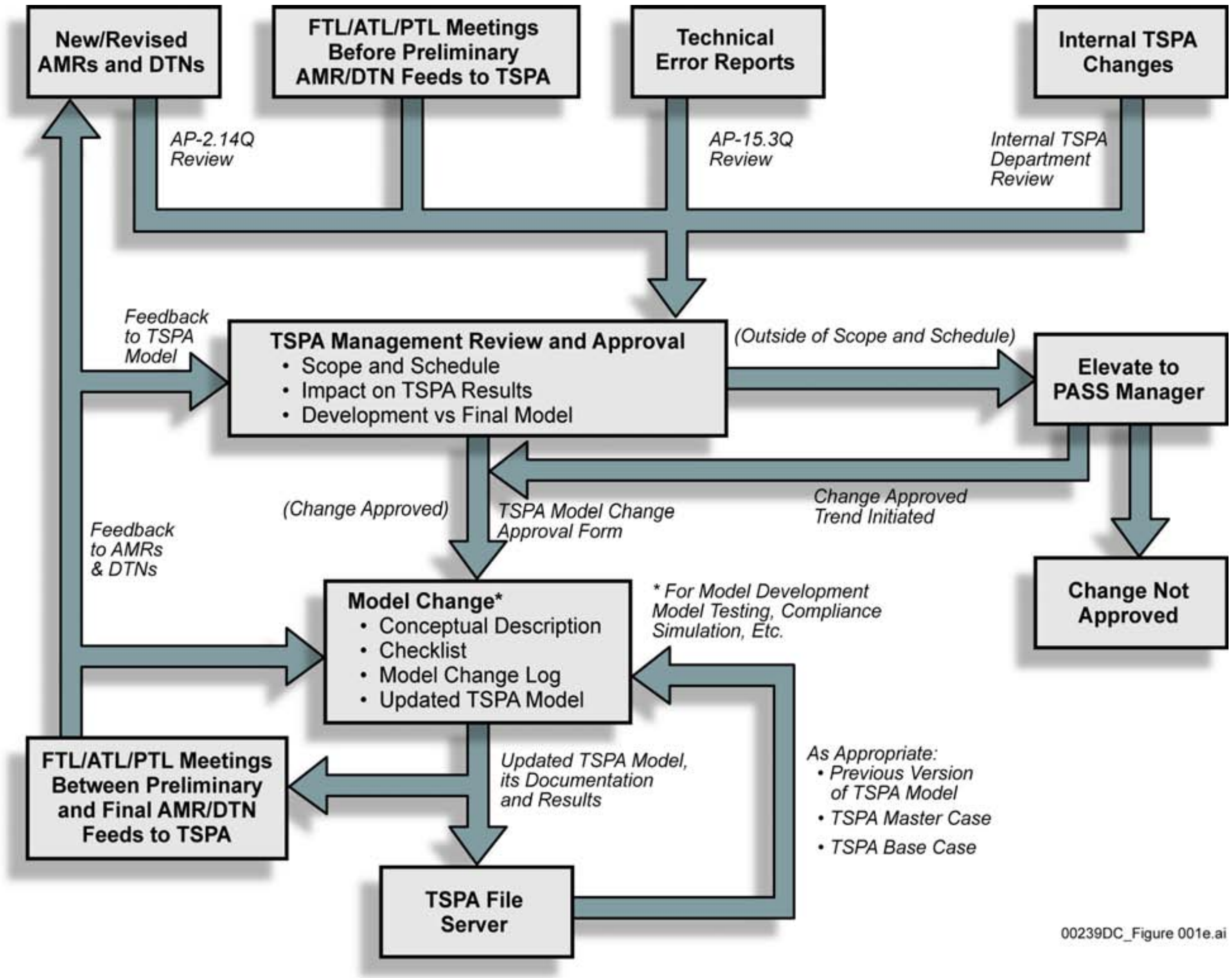


Figure 6.2-1. Flowchart Illustrating the Management Control Process for the TSPA-LA Model

TSPA Model Change Approval Form **QA: ___**

1. Change Number:
2. Basis for Proposed Changes(s):
3. Description of Proposed Change(s):
4. Expected Date of Change:
5. Is the change after the "frozen" date for the TSPA-LA model? __________
6a. Approve Change(s) ________ 6b. Disapprove Change(s) ________
7. Donald A. Kalinich, TSPA Model Calculations Group Lead Signature: Date:
8. John F. Pelletier, TSPA Configuration Management Lead Signature: Date:
9. Jerry A. McNeish, TSPA Department Manager Signature: Date:
10. Peter Swift, PASS Manager (signature required if change is after the TSPA-LA model freeze date) Signature: Date:

Figure 6.2-2. Example TSPA Model Change Approval Form

QA: ___

Case:
Starting Case:

Analyst:
Checker:

Parameter/Element/ Etc.	Location	Description of Change	Source	Checker Initials

Figure 6.4-1. Example TSPA Model Checklist

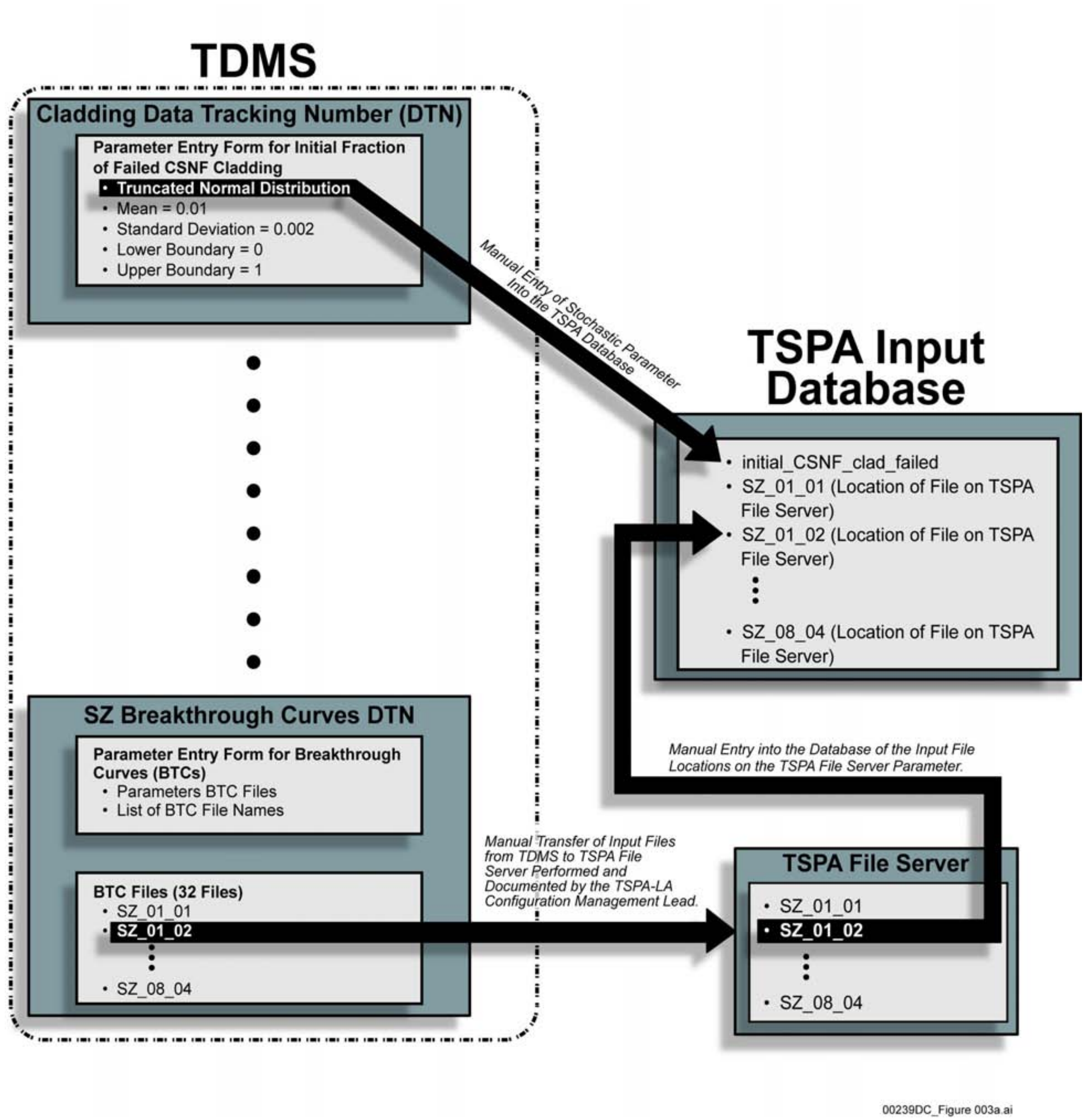


Figure 6.5-1. Illustration of Information Flow among the TDMS, TSPA File Server, and TSPA Input Database

QA: ___

Plot Name:

Analyst:
Checker:

Case	Element Plotted	Data Columns for Plot	Checker Initials

Additional items to check:

Are the time scales correct for each data set?

If the data sets are labeled in the data table, are they labeled properly?

Have all cases plotted been noted on the plot?

Is the name of the plot file noted on the plot?

Are the axis labels correct?

Is the legend correct?

If appropriate, is the plot disclaimer shown?

Figure 6.6-1. Example TSPA Plot Checklist

7. TSPA-LA MODEL VALIDATION

Validation of the TSPA-LA model is an important part of developing understanding and confidence in the model. It is important to note that validation refers to models, whereas verification refers to computer codes used to implement these models. Only the former is discussed in this section. Overall, the validation process is implemented and controlled by AP-SIII.10Q, *Models*.

This section provides an overview of the key aspects of the TSPA-LA model and its validation, including specific actions to be taken to enhance confidence (Section 7.1 and 7.2) and demonstrate stability and reliability of the statistical aspects of the numerical model (Section 7.3).

7.1 THE MODELING PROCESS: AN OVERVIEW

Validation of a computer model of a physical system involves a series of steps taken during and after the development of the model, designed to generate and enhance confidence in the predictions of the model. The modeling process starts from the modeler's understanding of the true physical system (the reality). A conceptual model is then formulated using simplifications, assumptions and some idealizations, and is translated into a mathematical model and subsequently to a numerical model. An appropriate computer code is selected to implement the numerical model. The inputs to the code are prepared and the code is executed to obtain the model predictions. This process is illustrated in Figure 7.1-1.

7.1.1 Conceptual, Mathematical, and Numerical Models

The first step in generating confidence in the model predictions consists of ensuring that the conceptual model captures the features of the physical system relevant to performance prediction; and that the idealizations, assumptions, and simplifications introduced result in a model that is appropriate for its intended use. In a similar way, the mathematical model should be adequate to represent the key processes in the conceptual model. The process of selection of input parameters and/or data, and the characterization of their associated uncertainties, should be documented in a way that generates confidence in the model development activity. The numerical model should include the proper level of discretization from considerations of precision, convergence, and stability (model calibration). Establishing model-to-reality conformity is the first step in validation. This conformity should be established separately for the conceptual, mathematical and numerical models. Documentation of all considerations leading to the formulation of the conceptual, mathematical, and numerical models and their calibration (in the AMRs), including the justification of assumptions, simplifications, and idealizations, should lend validity to the model formulation stage. Technical review of these models, in their formulation stage, would be considered as a step in the direction of model validation.

7.1.2 Computer Code and Associated Inputs

Converting the numerical model to a set of computer code algorithms is a process that must be transparent and traceable. Links from the numerical model to the computer code should be documented to permit easy checks on input construction. All inputs should be checked, controlled, and documented (see Sections 6.2 and 6.5). This process of checking the computer code construction and the associated inputs aids in establishing the validity of the model during the model-development stage (see AP-SIII.10Q, *Models*, Sec. 5.4.1b). Computer code verification itself, to ensure that the code implements the numerical model correctly, is controlled by AP-SI.1Q, *Software Management*.

7.1.3 Model Predictions: Corroboration with Independent Data

From a strictly computational perspective, a proper numerical model and a correct computer code should result in correct model predictions. However, it is not easy to demonstrate that a numerical model is an adequate representation of the complex physical system. To compensate for this difficulty, the final step in validation requires that the model predictions should be established as plausible and reasonable by corroboration with data from an independent source. This last step may be designated as model prediction validation.

However, the model prediction validation is not a trivial task. In the conventional modeling practice, prediction validation is achieved by comparing model predictions with experimental measurements. However, since these measurements would be impossible to obtain at the temporal and spatial scales of interest for postclosure performance, one or more of the seven alternative approaches listed in Section 5.4.1c of AP-SIII.10Q, *Models*, will be used to demonstrate prediction validation. The seven approaches are listed here for convenience:

- Comparison of model with data (not calibration)
- Comparison of results with alternative mathematical models
- Comparison with data published in refereed journals
- Peer review
- Technical review by independent reviewers
- Comparison of abstraction results to process models
- Comparison of pre-test model predictions to data collected during associated testing.

7.1.4 Different Stages of Model Validation

Based on the steps described above, the model validation activities are shown in Figure 7.1-2. These activities can be formulated as three separate stages, in the logical sequence of: (1) the input, (2) the code, and (3) the outputs of the model. Stage 1 relates to the validation of the model formulation stage including the selection of inputs and addressing the issues of convergence and stability of the model (calibration issues). Stage 2 addresses the mechanical issues of code verification and the construction of error-free inputs. Stage 3 addresses the validation based on the model outputs (predictions). Accordingly, this stage includes both the confidence-building activities recommended in AP-SIII.10Q, Sec. 5.4.1b, and the post-developmental activities by comparison with independent data as recommended in AP-SIII.10Q, Sec. 5.4.1c.

- **Stage 1: Model Formulation Validation/Calibration**–Show that the conceptual, mathematical and numerical models represent the physical system. Document the process of selection of the input parameters and/or data (and their uncertainties). Also, document the numerical model calibration activities to demonstrate the convergence and stability of the model. These steps generate confidence in the model (AP-SIII.10Q, Sec. 5.4.1b).
- **Stage 2: Computer Code and Inputs Verification**–Show that the computer code is verified thoroughly. Show that the input construction is error-free.
- **Stage 3: Model Prediction Validation**–Corroborate the model predictions with data from independent sources (AP-SIII.10Q, Sec. 5.4.1c). This stage includes confidence building activities, such as simplified test cases, as per AP-SIII.10Q, Sec. 5.4.1b. The rationale for combining some of the activities under both Sec. 5.4.1b, and Sec. 5.4.1c of AP-SIII.10Q lies in the fact that they both call for scrutiny of the model outputs. In contrast, Stage 1 scrutinizes the model inputs and model formulation.

When all the above three stages are completed, the model may be considered validated, so that its predictions could be used with confidence in assessing the performance of the physical system.

7.2 THE TSPA MODEL: VALIDATION

7.2.1 Stage 1: Model Formulation Validation/Calibration

The TSPA model is comprised of a linkage of several model components. The supporting AMRs document the validation of the underlying process models and/or abstraction models, including all the three stages cited in Section 7.1.4. In principle, each of these models is already validated before being integrated with the other models under the control of the TSPA-LA model computer code, GoldSim. It would therefore appear that the TSPA model will have *ipso facto* passed through Stage 1 (formulation of the conceptual, mathematical and numerical models) of the validation, subject possibly to a few caveats, as described below.

For example, the documentation for the process of selection of the model component input parameters and/or data, including their uncertainties, will be included in the relevant model document, and not in the TSPA-LA Model Document. However, it is conceivable that the combination of model components coupled together in the TSPA-LA model might generate conditions such that one or more model components produces output beyond the validated range documented in the model document. This will be examined as part of the TSPA model validation effort. Other conditions specific to the TSPA model, such as spatial, temporal, and stochastic discretization, convergence, and stability (see Section 7.3 and Appendix E) should also be checked as part of both development and post-development activities. These and other

TSPA model calibration activities will be documented in the TSPA-LA Model Document. Proposals for demonstrating convergence and stability of the stochastic aspects of the TSPA model are discussed in Section 7.3. A final point is that a few of the TSPA model inputs are specific to the system model, such as timestep length and others (see Section 6.5), and these will be documented in the TSPA-LA Model Document.

7.2.2 Stage 2: Computer Code and Input Verification

The purpose of this stage is to verify the suite of software codes and their associated input files as they implement the integrated TSPA model. Since all the component process models and other abstracted models will be validated for LA through all the stages (as documented in the different AMRs), Stage 2 of validation, (i.e., the code verification) has to demonstrate that all mechanical aspects of integrating the component codes are free from errors. Also, the construction of inputs within GoldSim must be shown to be error-free (see Section 6, also).

Step 1: Verification of the Integrated System Computer Code: GoldSim–The integrated system code, GoldSim, is fully verified by the code vendor, Golder Associates. It will also be qualified for use in TSPA in accordance with AP-SI.1Q, *Software Management*.

Step 2: Verification of DLLs as Single Modules in GoldSim–Some of the abstraction models within the TSPA-LA total system model will be implemented as DLLs, which are separately compiled and linked modules or subroutines that can be called by GoldSim—good examples being the waste package degradation software module WAPDEG and the UZ transport software module FEHM. The DLLs will be qualified by their developers, both from the standpoint of being correct representations of their underlying conceptual and mathematical models, and in terms of their mechanical operation as a DLL. Since the ability to properly call DLLs is a feature for which the GoldSim is qualified, DLLs qualified as previously described will, by default, be qualified to be called from within the TSPA-LA GoldSim model file.

Step 3: Verification of DLLs in the Integrated Model–There are two aspects to verification of all of the TSPA DLLs in the full TSPA-LA model. The first deals with the potential of two or more DLLs to conflict with each other in terms of memory requirements, duplicate input or output file unit numbers, etc. The second regards the potential interactions between DLLs (e.g., an output file generated by DLL "A" is used as an input file by DLL "B"). The appropriate test cases will be run and documented during model development to ensure that these types of verification issues are properly resolved.

Step 4: Verification of Inputs–Inputs to the TSPA model are controlled by the TSPA Input Database (see Section 6.5). Input parameters will be manually extracted from DTNs stored in the TDMS. The parameter entry forms in a DTN submittal will be used to locate the parameters in the DTN. Parameters entered into the TSPA Input Database will be checked and verified against their source DTNs.

Step 5: Verification of Single Model Components–The model components in the integrated TSPA model will have already been validated prior to implementation into the TSPA model.

Verification of proper implementation in the TSPA-LA model will be performed for each model component.

Step 6: Verification of Coupling between Model Components–The information transfer between connected model components will be verified. At this point, with the individual model components also validated and verified, it logically follows that the combination of coupled models are verified and validated.

7.2.3 Stage 3: Model Prediction Validation

Prior to this stage of validation, the input construction, the coupling of the model components, and the internal data transfers are all proven to be correctly handled in the TSPA model. The final phase of validation involves comparing model predictions with independently collected data.

Since, in general, the data cannot be observed on the real system (i.e., the combined natural and engineered systems modeled in the TSPA) at the times of interest (e.g., at 10,000 years after repository closure), conventional validation methods may not be applicable. One or more of the seven approaches recommended in AP-SIII.10Q, *Models,* and listed in Section 7.1.3 will be utilized for model prediction validation, as described in Section 7.2.3.2 below. Of these seven, the candidates to be used for the TSPA-LA model are: (1) comparison with alternative mathematical models, and (2) technical review by independent reviewers.

7.2.3.1 Confidence-Building Activities

Prior to the post-development validation activities using the approaches in Section 5.4.1c of AP-SIII.10Q, *Models*, a series of confidence-building activities will be performed, as indicated in Section 5.4.1b of AP-SIII.10Q, *Models*. These activities include such things as simple test cases (simplified inputs), analysis of selected deterministic realizations (e.g., a "median-like" realization), sequential "one-on" barrier analysis, and barrier neutralizations. These types of simulations help to test the different model components and their interactions within the total system model and they offer an enhanced understanding of the performance of the system and its parts, including an understanding of causal relationships, which in turn generates confidence in the entire TSPA model.

Simplified Test Cases–A sequence of simplified TSPA model components will be developed and tested within the framework of the TSPA-LA total system model. For example, at one extreme, one may consider a single waste package, with a failure resulting in a "constant" release rate of a single radionuclide, over a specified duration. The released radionuclide can be tracked through the different components (the EBS, UZ, and SZ) and mass conservation can be demonstrated. It is possible for this special case to check the model predictions with either alternative analytical solutions, or "back-of-the-envelope" calculations. Based on these results, the credibility of model predictions can be established. Table E.1-2 provides some examples of the model simulations in this category.

Single Deterministic Realizations: Median- and Higher-Dose Realizations–The compliance measure for Yucca Mountain is a mean time history of the repository performance averaged over multiple possible futures of the system performance (preamble to 10 CFR Part 63 (66 FR 55732 [156671], p. 55752)). Recognizing that cause-effect relationships are sometimes difficult to discern from such a "composite" measure of performance, several individual deterministic realizations will be evaluated to explicitly demonstrate causality in the total system model. Specifically, a single realization close in value to the median-dose time history (based on the multiple-realization runs) will be scrutinized and the releases from the components will be rationally explained. A study of the cause-and-effect relationships among key model components will be presented. This technical narrative should generate additional confidence in the TSPA model. A similar presentation will be made for a realization close in value to the 95th percentile (higher-dose) time history. The last entry in Table E.1-2 refers to this type of simulation.

Sequential One-On Barrier Simulations–These are stylized analyses that are designed to show understanding of system behavior and relative contribution of various barriers. The purpose of these analyses, similar to Electric Power Research Institute (EPRI)'s Hazard Index analyses (EPRI 2002 [158069]), is to provide rough, quantitative estimates of the importance of various barriers and processes (or combinations thereof) in reducing the potential hazard due to the emplacement of radioactive wastes at Yucca Mountain. The approach is to artificially "turn off" the function of all barriers and processes initially, and then add them back sequentially in some logical order (e.g., waste form barriers first, natural barriers second, and engineered barriers last). These studies are expected to offer an in-depth understanding of the system and thus build confidence in the validity of the TSPA-LA model.

Table E.3-1 contains examples of one set of sequential one-on barrier/FEPs simulations for the nominal scenario class. Additional one-on simulations may be run for the igneous groundwater release scenario and the seismic scenario class. Also, the barriers/FEPs could be added in a different sequence, and different treatments of the barriers/FEPs could be considered.

Barrier/Process Neutralizations–In a neutralization analysis, the fundamental idea is to examine the extent to which performance of the overall system is degraded if the ability of a given barrier to perform as expected is compromised. As such, the approach precludes reliance on complete knowledge of any one process. This increases confidence that the postclosure performance objectives, as specified in the regulations, will be met.

The TSPA-LA model will first be evaluated for the base case with all the barriers performing as expected (including their uncertainties). In the next step, each barrier is neutralized one at a time (i.e., the barrier is assumed to be absent and/or performing at very pessimistic levels). In other words, the barrier is physically in place, but its ability to retard and/or attenuate water and/or radionuclide movement is completely ignored. The performance of the neutralized system is computed and compared against that of the base case.

Examples of barrier/process neutralization simulations are provided in Table E.4-1. They would be performed for both the nominal and igneous groundwater release base cases. Barrier/process neutralization simulations may also be developed for the igneous eruptive release and seismic modeling cases. Also, different ways of neutralizing the barriers/processes could be considered, and additional processes/barriers could be considered.

As in the case of sequential one-on analyses, these studies are expected to offer an in-depth understanding of the system and thus build confidence in the validity of the TSPA-LA model.

7.2.3.2 Model Prediction Validation Approaches

This section describes in more detail some of the approaches that may be used from Section 5.4.1c of AP-SIII.10Q, *Models*—the "post-development validation activities."

Comparison with Alternative Models–The TSPA-LA model predictions may be compared directly to similar results from other well-established models, such as EPRI's IMARC model (EPRI 2002 [158069]) and NRC's TPA model (NRC 1999 [152183]), if they are updated to the TSPA-LA model inputs (as per AP-SIII.10Q, Sec. 5.4.1c). The uncertainty range for dose results from the DOE TSPA and the EPRI and/or NRC models could be compared, if the corresponding inputs are similar. The comparison is not currently applicable to the DOE TSPA-LA model (still under development), but could be made with a precursor model such as the TSPA-SR or TSPA-FEIS model that may have formed the basis for either a published EPRI model or a published NRC model. A cdf, pdf, or box plot for dose from these various models could be compared. A reasonable overlap may be considered to provide further evidence of the validity and/or robustness of the DOE TSPA model predictions. In order to use such a comparison based on the TSPA-SR or TSPA-FEIS models, for validation of the TSPA-LA model, it would be necessary to evaluate how much had changed from the earlier TSPA model to the TSPA-LA model, to see how much significance could be placed in this comparison.

Technical Review–Another method of validation is to subject the model predictions to an intense scientific review (technical review per AP-2.14Q), where the reviewers study the model and its predictions critically and identify any "implausible" results or loop-holes in the analysis and offer suggestions to correct those situations. This type of careful scientific scrutiny will be used as a validation methodology.

It should be mentioned that the TSPA-SR method, which is a precursor to the TSPA-LA, has been subjected to a peer review by an OECD/NEA-IAEA International Review Team (OECD and IAEA, 2002 [158098]). To quote from their findings:

> "…the TSPA-SR methodology is soundly based and has been implemented in a competent manner…Overall the IRT considers that the implemented performance assessment approach provides an adequate basis for supporting a statement on likely compliance within the regulatory period of 10,000 years…"

The International Review Team also recommended a number of improvements and changes to result in more confidence and robustness in the TSPA model. Given the favorable review by an international review panel, this should generate confidence in the validity of the TSPA-LA model, which will evolve from the TSPA-SR model.

7.3 STABILITY AND RELIABILITY OF TSPA MODEL RESULTS

In TSPA-LA, Latin hypercube sampling (LHS) (McKay et al. 1979 [127905]) will be used in the propagation of uncertainty. This sampling technique has been selected, as in past TSPAs, because of the efficient manner in which it stratifies across the range of each uncertain variable and the observed stability of uncertainty and sensitivity analysis results obtained in past applications of LHS in performance assessments for complex systems (McKay et al. 1979 [127905]; Iman and Helton 1991 [159039]; Helton 1999 [159042]). Here, stability relates to how much variability takes place in the outcome of interest as the model results are repeatedly calculated with different samples. Theoretical results indicate that, under certain conditions, LHS does indeed exhibit better statistical convergence properties than random sampling (McKay et al. 1979 [127905]; Stein 1987 [159060]). However, these results are difficult to apply in practice. As a result, a practical method of assessing the stability of results obtained with LHS is needed.

The main issue regarding stability of the TSPA model results is whether enough Monte Carlo runs have been performed to adequately quantify the uncertainty in the dose estimates. The OECD-IAEA International Review Team expressed concern on this issue (OECD and IAEA 2002 [158098]). The NRC identified the stability of the TSPA model results as a Key Technical Issue (KTI) agreement item (i.e., TSPAI 4.03 (Meserve 2001 [156977]), as described in Appendix B). Section 4.2.1.4 of the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) specifically mentions the stability of the TSPA-LA model results as an acceptance criteria, stating:

> "A sufficient number of realizations has been obtained, for each scenario class, using the total system performance assessment code, to ensure that the results of the calculations are statistically stable."

Another concept associated with the probabilistic model calculations is the reliability, or confidence, in the mean dose estimates. The stability and reliability of the TSPA-LA results, produced to demonstrate regulatory compliance, are important to validation and confidence building (as per AP-SIII.10Q, Section 5.4.1b) and are the subject of the discussion presented in this section. For the purposes of this discussion of statistical convergence of TSPA-LA model results, the following definitions will be used:

- **Stability** – refers to the sensitivity of expected dose to sample size, and is therefore a reflection of the "accuracy" of the Monte Carlo simulation methodology.

- **Reliability** – refers to the uncertainty in estimates of the expected dose, and is therefore a reflection of the "precision" of the Monte Carlo simulation methodology.

The stability question can be answered by running the model multiple times with a different number of realizations each time, and examining the convergence behavior of the expected dose. The reliability question can be answered by computing the confidence intervals for the estimated value of expected dose.

The exact approach to be used for investigating stability and reliability of the TSPA-LA model has not been finalized. However, some of the techniques under consideration are described in the following sections. These techniques are drawn from previous TSPA studies, other radioactive waste performance assessment programs (e.g., Waste Isolation Pilot Plant (WIPP), Atomic Energy of Canada, Ltd (AECL)), as well as the probabilistic risk analysis literature.

7.3.1 Tests for Stability

As noted earlier, stability refers to the sensitivity of model results to sample size. Quantification of the stability of model results involves carrying out multiple model runs with a different number of realizations each time, and examining how the computed outcomes appear to converge on some constant value. Note that this is the value that would have been obtained with an infinite number of realizations. However, practical considerations allow only a finite number of realizations to be used – hence the need to deal with the issue of stability or statistical convergence.

Approaches proposed for evaluating the stability of model results involve graphical comparisons of model output at various sample sizes, performing statistical tests to evaluate if the expected dose obtained with two different sample sizes are the same or different, and performing statistical tests to evaluate if the distributions of dose obtained with two different sample sizes are the same or different. These approaches are briefly summarized below.

(a) Graphical comparison - The simplest test for stability involves examining a graph of the computed model outcome (e.g., expected dose) versus sample size. Alternatively, for time-dependent problems, the model outcomes for different sample sizes can be overlain on the same graph to facilitate a comparative analysis. This is the approach followed in TSPA-SR, where a visual examination of results was performed to assess whether an adequate number of realizations was performed. Specific percentiles (e.g., 5th, 50th, 95th percentiles) of the output data were calculated for a suite of model runs and compared. The suite of model runs included 300-, 500-, and 1000-run simulations of the nominal TSPA model. In addition, several 300-run simulations were performed with different random seed numbers for the LHS sampling. As pointed by the NRC and others (e.g., KTI agreement TSPAI 4.03 (Meserve 2001 [156977]); OECD and IAEA 2002 [158098]) such simple tests need to be supplemented by quantitative measures to define the adequacy of the number of model runs in the TSPA calculations.

(b) Testing for difference in mean - The difference in mean doses obtained from samples of two different sizes can be tested for statistical significance. The difference in the mean dose can be small, but can be significant, if the sample size is large. Similarly, the difference can be large, but not significant, if the sample size is small. A quantity that measures the significance of the difference of means is based on the standard error (sample standard deviation divided by the square root of the sample size). The standard error measures the accuracy with which the sample mean estimates the "true" mean. In this approach, a Student-t is computed based on the standard error of the difference of the means (Press et al. 1992 [103316]) and the significance of the difference is evaluated, using the *t* distribution. An appropriate level of significance (e.g., 1% or 5%) is chosen to ensure that the means are not significantly different. A significant difference between the means suggests that the smaller sample size, and possibly the larger sample size as well, is providing an inadequate estimate of the mean.

(c) Testing for difference in distributions: In order to assess if two different distributions are statistically alike, i.e., there is no significant shift in the magnitude of the values of the distributions (i.e., larger or smaller values), a statistical ranking test may be performed. One such test is the Wilcoxon Rank Sum test (Walpole et al. 1998 [152180])). In order to apply the Wilcoxon Rank Sum test to evaluate the similarities between two distributions (e.g., 300-run vs. 1000-run simulations at a particular output time), the two data distributions are combined and ranked from lowest to highest values. Next, the rankings from one of the two distributions are summed. The rank sum is then used in a mathematical formulation to compute a Z statistic, which is compared to a tabulated Z statistic for an assumed significance level to determine if the distributions are statistically different or alike.

The two tests described above for verifying whether the means are similar and whether the distributions are similar can also be used in conjunction with the methods described in the next section (for estimating the confidence in estimates of the mean) to provide a consistency check on the identification of the smallest sample size that appears to produce statistically stable estimates of the expected dose.

7.3.2 Tests for Reliability

To assess the reliability, or confidence, in the mean dose results, it is appropriate to calculate confidence intervals about the mean. Uncertainty in the mean of a distribution, which is caused by the use of a finite sample size can be represented by a sampling distribution (Cullen and Frey, 1999 [107797]). A variety of methods are available for characterizing uncertainty in the sample mean of a distribution, each based on a different assumption regarding the sampling distribution. Some of these methods are discussed next, and address KTI agreement TSPAI 4.05 (Meserve 2001 [156977]).

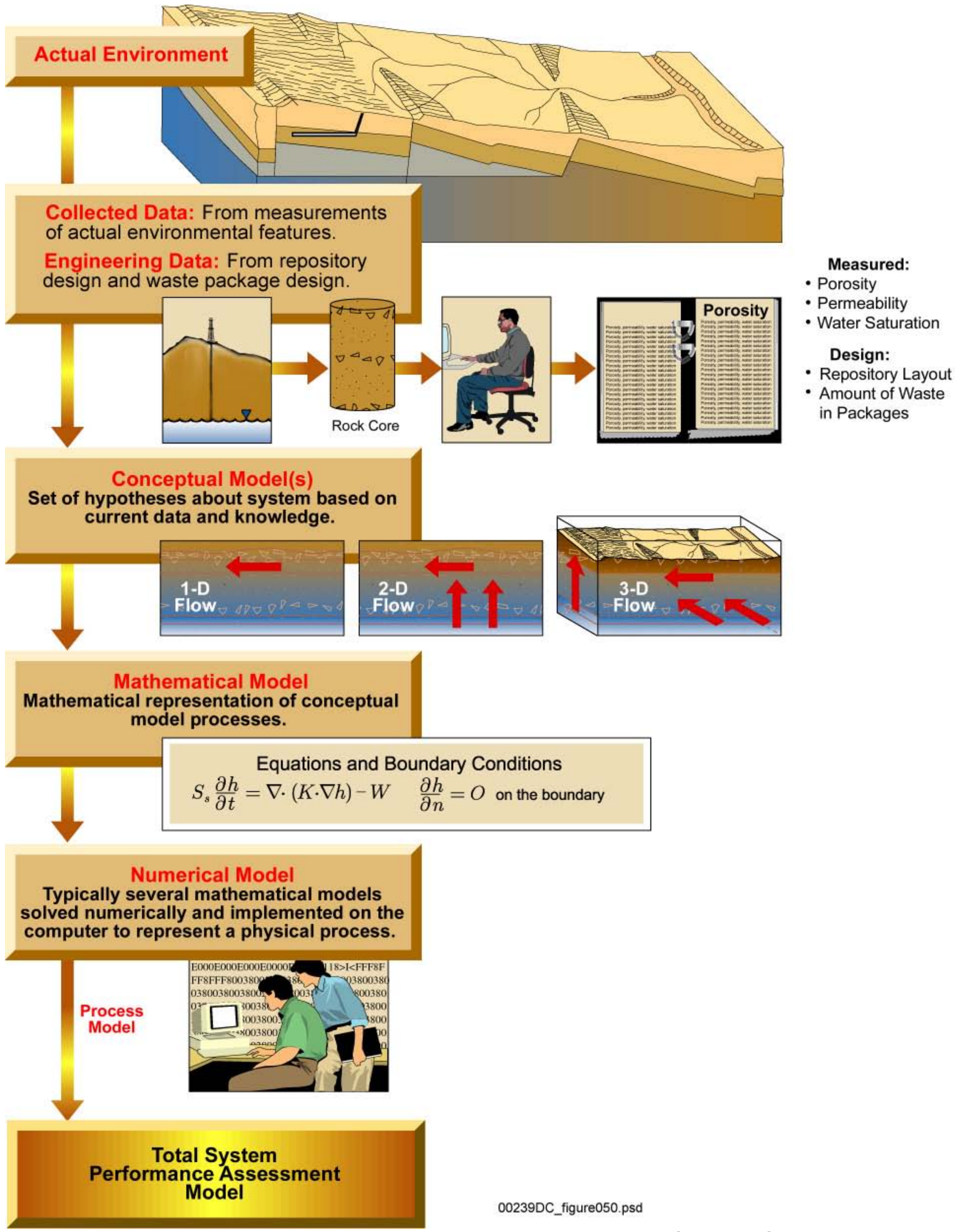
(a) Central limit theorem – A well-known result from statistics, the central limit theorem, states that if the sample size, n, is reasonably large, no matter what the distribution of x, the sample mean will be approximately normal (Benjamin and Cornell, 1970 [110221]). Once the mean and its standard deviation have been computed, estimates of reliability (such as 95% confidence intervals) can be obtained using the properties of the normal distribution.

(b) Sub-sample analysis – In this approach, the sample set is divided into a smaller number of sub-samples, and the mean computed for each of these sub-samples. Thus, an approximation of the sampling distribution of the mean is created. Next, the mean of the means, and the standard deviation of the means, is used in conjunction with the properties of the t-distribution to obtain the 95% (or any other desired) confidence interval. Such an approach was used in the 1994 AECL performance assessments to determine the confidence associated with the expected dose at selected points in time (Goodwin et al. 1994 [124152], Section A.3.5). It should be pointed out that a random sampling scheme was used in the AECL performance assessment study, as compared to the LHS scheme to be used in TSPA-LA.

(c) Replicated sampling – A replicated sampling procedure developed in the NRC's high level waste program at SNL provides an effective approach to estimating the potential sampling error in quantities derived from LHS (Iman 1982 [146012]). With this procedure, the LHS is repeatedly generated with different random seeds. These samples are used to produce a sequence of values for the expected dose, from which its mean and standard error are computed. Confidence intervals for the expected dose can then be estimated with the *t*-distribution. The appropriate value for the number of replicates cannot be known with assurance before an analysis because the size and location of the resultant confidence interval will depend on both the mean and standard error. For example, a much wider confidence interval might be acceptable if the expected dose was much less than a regulatory outcome of concern than would be the case if it was close to a regulatory outcome of concern. In practice, a reasonable computational strategy is to start with a small number of replicates (e.g., 3-5), and then add additional replicates if the initial confidence interval is too close to an outcome of concern.

(d) Bootstrap – Bootstrap simulation is a numerical procedure for simulating the sampling distribution and estimating its mean, standard deviation and confidence intervals associated with such quantities. Cullen and Frey (1999 [107797]) describe the percentile-bootstrap method, known as bootstrap-*p*, to estimate confidence intervals for the mean of a distribution. Given a data of sample size *n*, the general approach in bootstrap simulation is to: (1) assume a distribution which describes the quantity of interest, (2) perform *r* replications of the data set by randomly drawing, with replacement, *n* values, (3) calculate *r* values of the statistics of interest. In step 1, parametric models such as normal or log-normal distributions can be used to fit to the data, or the empirical distribution can be sampled by assuming that the data can be described by a cumulative distribution that is piecewise linear between each data point, or the actual data set itself can be resampled. Furthermore, confidence intervals for the mean can be readily obtained from the *r* values that form an approximation of its sampling distribution.

(e) Non-parametric bounds – When the underlying population distribution is not normal and a small sample of the distribution is available, then the normal distribution may not be a good approximation of the sampling distribution of the mean. A non-parametric method that has been used to compute confidence intervals, which does not require that the data are normally distributed, is the Tchebycheff inequality. Here, the confidence intervals around the mean are taken to be plus or minus some multiple of the standard error. However, the Tchebycheff method produces significantly larger estimates of the confidence limits as compared to the normal distribution. An improvement on the Tchebycheff inequality was developed by Guttman (Woo 1989 [159073]). The multipliers for the Guttman inequality method are larger than the normal bound coefficients, but significantly smaller than the Tchebycheff coefficients. For instance, at a 95% confidence bound these multipliers for the normal, Guttman, and Tchebycheff methods are 1.96, 2.68, and 4.47, respectively. The Guttman inequality can be used to provide bounds on the confidence limits generated with such methods as the bootstrap or replicated sampling which attempt to recreate the sampling distribution.



Source: DOE 1998 [100550], Figure O-2

Figure 7.1-1. Generalized Performance Assessment Approach

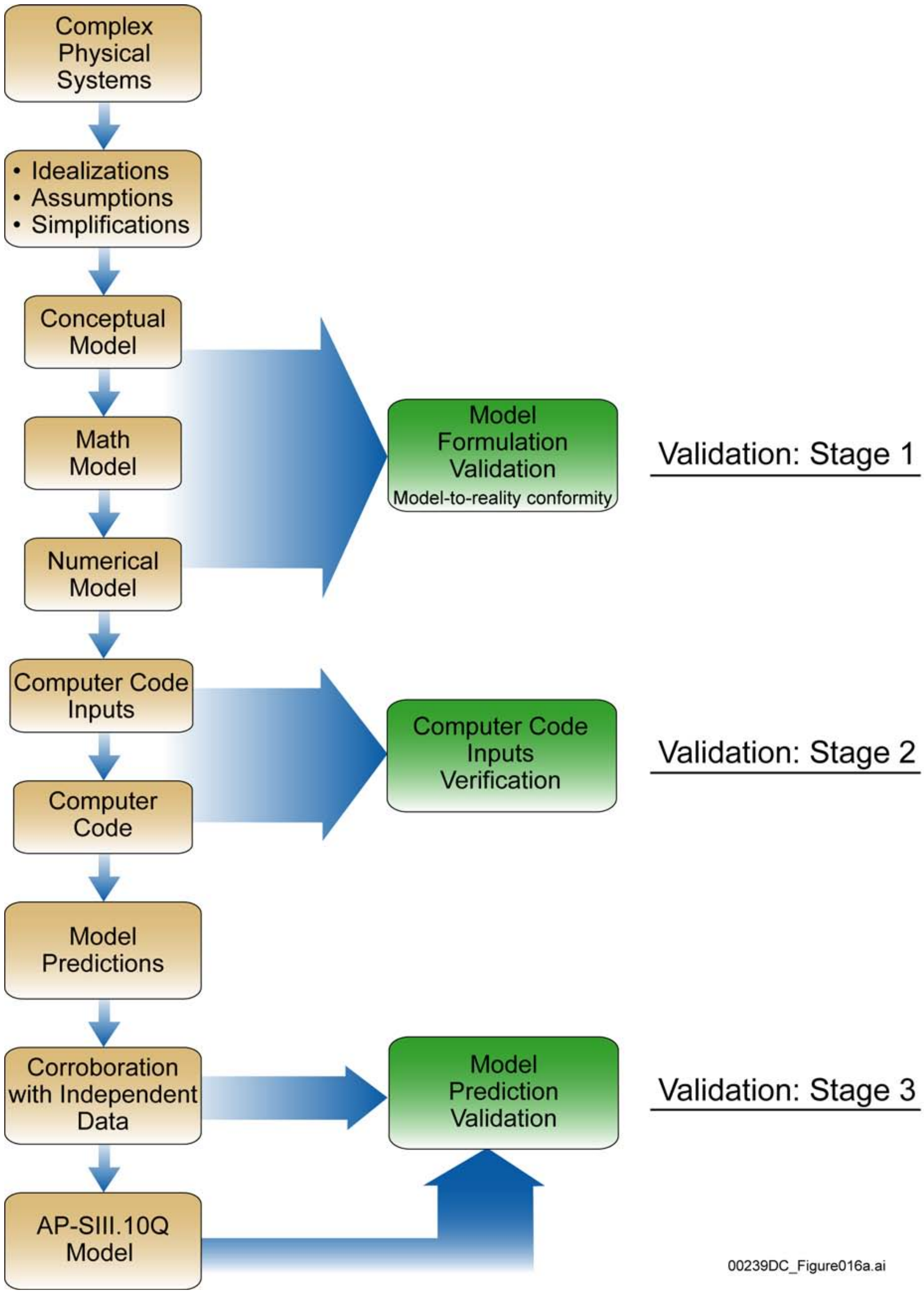


Figure 7.1-2. Model Validation Stages

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8. TSPA-LA ANALYSES

The analysis of the TSPA-LA will cover three broad topics. It will describe the uncertainties inherent in the model and how they are manifested in the results. This approach is described in Section 8.1. It will evaluate the sensitivity of the model through a variety of techniques. This approach is described in Section 8.2. The analyses will also support the development of a description of barriers and their capabilities from the perspective of the TSPA-LA model. This aspect, which is also important to satisfying the 10 CFR Part 63 requirements, is presented in Section 8.3. These analyses will be documented in detail in the TSPA-LA Analysis Document, a draft outline for which is provided in Appendix D.

8.1 APPROACH TO UNCERTAINTY ANALYSES

The probabilistic framework underlying the TSPA-LA calculations is based on the regulatory requirements described in Section 1.3. Briefly, multiple calculations will be carried out for each of the scenario classes described in Section 4, using sampled values of parameters representing the expected uncertainty range, to calculate the expected dose required for compliance analysis as per 10 CFR Part 63. The suite of simulations that will form this calculation set are presented in Appendix E. In this section, the focus is on the approach for describing the base-case simulation results. The base-case simulations are probabilistic calculations, carried out separately for each of the nominal, igneous and seismic scenarios classes. These simulations will be carried out in two steps: (a) covering the 0 to 10,000 year regulatory time period with results to be documented in the License Application, and (b) covering the 0 to 20,000 year period to demonstrate that the model results have no major changes after the regulatory time period. The methodology for interpreting results of these simulations is described below.

8.1.1 Nominal Scenario Class

The nominal scenario class contains a single modeling case that is composed of the set of expected FEPs, as determined by a formal FEP screening procedure described in Section 3.2.2. The nominal scenario class for TSPA incorporates the important effects and system perturbations caused by climate change and repository heating that are projected to occur over the 10,000-year compliance period.

The principal model components of the TSPA-LA, listed in the general order information is passed from model to model (as shown in Figure 5-2), include:

- Unsaturated zone flow
- Engineered barrier system environment
- Waste package and drip shield degradation
- Waste form degradation and mobilization
- Engineered barrier system flow and transport
- Unsaturated zone transport

- Saturated zone flow and transport
- Biosphere.

The nominal scenario class exercises these component models to describe the anticipated sequence of processes that are expected to occur during the lifetime of the proposed repository. A more detailed description of the processes included in the nominal scenario class can be found in Section 5.1.

Results of the nominal scenario class will be analyzed at the total-system and the subsystem level. Analyses of total system results will be based on the expected dose metric, and will include analysis of one or more of the following:

- Time history plots of the expected dose, along with running 5th, 50th, and 95th percentile curves. Dose-time history from all of the individual realizations will also be presented in the form of a "horsetail plot"
- Key radionuclides and their contributions to expected dose
- Side-by-side histogram of dose at selected times, showing the temporal evolution of dose distribution and the frequency of extreme outcomes
- Side-by-side histogram of time to reach specified dose, showing the performance of the system in comparison to regulatory dose and time limits.

Analyses of subsystem results will be based, among other things, on metrics related to the integrity of engineered components and will include analysis of one or more of the following:

- Cumulative drip shield failures
- Cumulative waste package failures
- Waste package opening area
- Water flow rates into drift, through the drip shield and into waste package
- Fractional cladding failures.

Additional subsystem metrics include those related to the movement of radionuclides through the system, such as:

- Mean release rates for a variety of key radionuclides representing different combinations of sorption potential and solubility characteristics. These results may be presented for the waste form, the waste package, EBS, UZ, and SZ subsystems.
- EBS release rates may be further analyzed in terms of release process (e.g., advective versus diffusive) and waste types (e.g., CSNF and codisposal waste).
- UZ and SZ releases may be further analyzed in terms of spatial discretization (e.g., infiltration bins) and spatial location (e.g., mass collection regions).

Figures 8.1.1-1 through 8.1.1-12 present illustrations of how the performance of the total system and various subsystems will be represented to highlight the various metrics discussed above. These analyses will be carried out in terms of the expected value of the appropriate metric. In addition, the spread around the mean for each of the metrics will be presented at selected times in the form of side-by-side box plots to indicate the uncertainty in projected outcomes. Figures 8.1.1-1 through 8.1.1-12 should not be construed as depictions of actual performance projections, rather they show illustrative examples of how the system response will be graphically presented.

8.1.2 Igneous Scenario Class

The volcanic eruption and igneous intrusion groundwater transport modeling cases are the two igneous activity modeling cases considered for TSPA-LA. These two modeling cases were described in Section 4 and are briefly recounted below.

The volcanic eruption modeling case will consider the direct transport of waste to the ground surface from the repository in a volcanic eruption. This modeling case will begin with an eruptive event, which will be characterized in the TSPA by both its probability and its physical properties such as energy and volume of the eruption, composition of the magma, and properties of the pyroclastic ash (Figure 5.3-1). Interactions of the eruption with the proposed repository will be described in terms of the damage to the EBS and the waste package. Characteristics of the waste form in the eruptive environment will be described in terms of waste particle size. Atmospheric transport of waste in the volcanic ash plume begins with entrainment of waste particles in the pyroclastic eruption and will be affected by wind speed and direction. The manner and details in which waste dispersion will be handled for the eruptive event are currently under review. The final detailed approach will be discussed in the appropriate AMR.

BDCFs will be developed for exposure pathways relevant to atmospheric deposition of contaminated ash, rather than for the groundwater pathways considered for nominal performance. As a final step, the volcanic eruption BDCFs will be used to determine radiation doses resulting from exposure to contaminated volcanic ash 18 km from the proposed repository.

The igneous intrusion groundwater transport modeling case will consider an igneous intrusion that travels down the drifts and remains underground. Although the intrusion damages waste packages and other components of the EBS, FEPs analyses have concluded that it does not significantly alter the long-term flow of water through the mountain (CRWMS M&O 2000 [151553], Section 6.2.16). As shown in Figure 5.3-2, the igneous intrusion groundwater transport model will use information about the probability of intrusion, the characteristics of the intrusion, and the response of the proposed repository to calculate damage to waste packages. Groundwater transport away from the damaged packages will be calculated using the nominal scenario class models, and doses to humans from contaminated groundwater are determined using nominal BDCFs.

Results of the igneous scenario class will be analyzed at the total-system and the subsystem level. Presentation of these results will be similar to the structure presented previously for the nominal scenario class. However, not all elements will need to be presented by virtue of the disruptive nature of the scenario class, which could eliminate certain barriers and/or transport pathways.

8.1.3 Seismic Scenario Class

The seismic scenario class considers seismic hazards that occur near the repository. Although the subsequent ground motion and fault displacement (if screened in) at the repository horizon damages waste packages and other components of the EBS, ongoing FEPs analyses indicate that these seismic hazards will not significantly alter the long-term flow of water through the mountain. This modeling case begins with a ground-motion event, which will be characterized in the TSPA-LA by its mean annual frequency and amplitude (see also Sections 4.3 and 5.3.2). This seismic hazard may cause damage to drip shields, waste packages, and cladding. Radionuclides are then released from damaged waste packages and subsequently transported by the groundwater to the biosphere. Groundwater transport away from the damaged packages will be calculated using the nominal scenario class models, and doses to humans from contaminated groundwater are determined using nominal BDCFs.

Results of the seismic scenario class will be analyzed at the total-system and the subsystem level. Presentation of these results will be similar to the structure presented previously for the nominal scenario class. However, not all elements will need to be presented by virtue of the disruptive nature of the scenario, which could eliminate certain barriers and/or transport pathways.

8.1.4 Combined Results

For compliance demonstration purposes, it is necessary to produce a quantitative result suitable for comparison with the regulatory limit. This requires that the probabilistic calculations of the expected annual dose histories for the nominal and disruptive scenario classes be combined through a probability weighting method, where the contribution of each scenario class to the expected dose is the product of the dose from that scenario class and its probability (the probabilities being as indicated in Table 4-1). This expected annual dose includes the likely performance of the disposal system (the nominal scenario class) and the consequences of unlikely events (disruptive scenario classes).

The probabilistic framework employed for the TSPA-LA calculations will produce multiple histories of annual dose for the nominal scenario class and each of the disruptive scenario classes. A Monte Carlo simulation technique will be used to incorporate uncertainty and variability in the model input parameters by using different vectors of sampled values for each realization. Therefore, results for each modeled scenario will include a separate dose history for each sampled vector. Dose histories for each input vector will be combined to produce a conditional mean dose history for each scenario. The use of the term "conditional" indicates that these are the mean doses expected if the chosen scenario conditions were certain to occur. Because the scenario probabilities partition the probability space, the conditional mean dose histories must be weighted by the scenario probabilities and summed to give the overall expected annual dose history.

8.1.5 Groundwater Protection Analyses

An analysis of groundwater protection will be conducted in accordance with the regulations at 10 CFR 63.331, 63.332, and 63.342. This analysis will consider likely features, events, and processes, i.e., those estimated to have a probability greater than one chance in 10,000 of occurring within 10,000 years of disposal. The analyses may consider some unlikely features, events, or processes, but in no case will they consider features, events, or processes not included in the nominal scenario class (e.g., igneous or seismic scenario classes). 10 CFR 63.331 sets limits on radionuclides in the representative volume of groundwater at the accessible environment for the first 10,000 years after repository closure. The limits for contamination within a representative volume of 3,000 acre-ft of groundwater are defined in terms of activity concentration per unit volume and dose, depending on radionuclide or type of radiation emitted.

Concentration Limits-There are two concentration limits defined. The combined activity concentration limit for radium-226 and radium-228 is 5 picocuries per liter. The gross alpha activity (including radium-226 but excluding radon and uranium) is 15 picocuries per liter. Both of these limits include contribution from natural background radiation sources (10 CFR 63.331) at the location of the RMEI.

In assessing compliance against these standards, TSPA will where possible, use the calculated concentration of the appropriate radionuclides. For those radionuclides included by the standard but not tracked explicitly in the TSPA model, it will be assumed that all progeny are in secular equilibrium with their tracked predecessor to determine their contributions to total activity concentration.

Dose Limit-The dose limit is defined as the total annual dose from the combined beta and photon emitting radionuclides. The limit defined by the standard is 4 mrem (0.04 mSv) per year to the whole body or any organ, based on drinking 2 liters of water per day from the representative volume (10 CFR 63.331). The representative groundwater volume is that which would be withdrawn annually from an aquifer containing less than 10,000 mg/L of total dissolved solids, and centered on the highest concentration in the plume of contamination at the same location as the RMEI (10 CFR 63.332).

TSPA-LA will calculate the concentrations of the contributing radionuclides in the representative volume in a manner consistent with the method used to demonstrate compliance with the groundwater protection standard in 10 CFR 63.311.

In determining compliance with the 4 mrem per year dose limit, the radionuclide dependent parameters will be dose conversion factors (committed dose equivalent per unit intake of a radionuclide) for the whole body and individual organs. These dose conversion factors for the ingestion pathway are provided in Table 2.2 of Federal Guidance Report No. 11 (Eckerman et al. 1988 [101069]). The algorithm used to calculate either the whole body dose or any organ dose is given by

$$D_i = \sum_{all\ j} D_{ij} \qquad \text{Eq. 8.1-1}$$

where

D_i is the annual dose (mrem/year) to whole body (*i=0*) or organ *i* from drinking two liters of water per day from the representative volume.

D_{ij} is the annual dose (mrem/year) from radionuclide *j* to whole body (*i=0*) or organ *i* from drinking two liters of water per day from the representative volume and is given by Eq. 8.1-2:

$$D_{ij} = w \times d \times DCF_{ij} \times C_j \qquad \text{Eq. 8.1-2}$$

where

w is the daily intake of drinking water prescribed in 10 CFR 63.312 (2 liters/day)

d is the number of days in a year (365.25 days/year)

DCF_{ij} is the dose conversion factor from Federal Guidance Report No. 11 (Eckerman et al. 1988 [101069]) for ingestion of radionuclide *j* for the whole body or individual organ *i* (mrem/Bq)

C_j is the concentration (Bq/liter) of radionuclide *j* in the representative volume of groundwater calculated by TSPA as prescribed by 10 CFR 63.332.

Based on Equations 8.1-1 and 8.1-2, the dose limit in Table 1 of 10 CFR 63.331 is

$$D_i \leq 4 \text{ mrem/yr, for all } i \qquad \text{Eq. 8.1-3}$$

TSPA will calculate the annual dose to the whole body and individual organs from the beta and photon emitting radionuclides tracked by TSPA and their decay products. For the radionuclides not tracked by TSPA but included in the groundwater protection standard, it will be assumed that all progeny are in secular equilibrium with their tracked predecessor in order to determine their contributions to annual dose.

8.2 APPROACH TO SENSITIVITY ANALYSES

The TSPA-LA model represents the behavior of a complex system with hundreds of parameters. Many of the parameters are uncertain and/or variable, and their interaction with one another can also be complex and/or highly nonlinear. It is difficult to obtain an understanding of exactly how the model works and what the critical uncertainties and sensitivities are from a simple evaluation of model results. To this end, sensitivity analysis provides a useful and structured framework for unraveling the results of probabilistic performance assessments by examining the sensitivity of the TSPA-LA model results to the uncertainties and assumptions in model inputs.

Sensitivity analysis, in its simplest sense, involves quantification of the change in model output corresponding to a change in one or more of the model inputs. In the context of probabilistic models, however, sensitivity analysis takes on a more specific definition, namely, identification of those input parameters (and their associated uncertainties) that have the greatest influence on the spread or variance of the model results (Helton 1993 [100452]). This is sometimes referred to as global sensitivity analysis or uncertainty importance analysis to distinguish it from the classical (local) sensitivity analysis measures typically obtained as partial derivatives of the output with respect to inputs of interest.

The contribution to output uncertainty (variance) by an input is a function of both the uncertainty of the input variable and the sensitivity of the output to that particular input. In general, input variables identified as important in global sensitivity analysis have both characteristics; they demonstrate significant variance and are characterized by large sensitivity coefficients. Conversely, variables which do not show up as important per these metrics are either restricted to a small range in the probabilistic analysis, and/or are variables to which the model outcome does not have a high sensitivity.

In the context of TSPA-LA, the goal of sensitivity analysis is to answer questions such as:

- Which uncertain variables have the greatest impact on the overall uncertainty (spread) in probabilistic model outcomes?
- How can significant input-output relationships be identified if the association between input-output pairs is nonlinear and nonmonotonic?
- Which are the key factors controlling the separation of model outcomes into higher-dose and lower-dose producing realizations?

TSPA-LA will use regression-based analyses, entropy-based analyses, and classification-tree-based analyses to answer these questions, respectively. Details of each of these methods are described in the following sections. The analyses will be carried out using results from the probabilistic TSPA-LA model calculations at a fixed point in time (e.g., at the time corresponding to the peak of the mean dose during the regulatory period). The sampled inputs corresponding to each of the realizations will be treated as independent variables and the computed outputs will be treated as dependent variables. The outputs can either be total system-level performance measures, such as annual dose rate to a RMEI, or they can be subsystem-level performance measures, such as cumulative radionuclide mass flux at the water table.

8.2.1 Regression-Based Analyses

The goal of regression-based analyses is to build a multivariate linear regression model between the output and the uncertain inputs in order to identify the strength of association between various input-output pairs (Helton 1993 [100452]). To this end, the variables are first rank transformed to linearize any underlying nonlinear trends and facilitate the application of linear regression tools. In the surrogate input-output model, the output variable is represented as a weighted linear sum of the uncertain inputs. The unknown weights (regression coefficients) are generally determined using a stepwise regression procedure as described below.

In the stepwise regression approach, a sequence of regression models is constructed starting with a single selected input parameter (usually the parameter that explains the largest amount of variance in the output). One additional input variable is included at each successive step (usually the parameter that explains the next-largest amount of variance). The process continues until all of the input variables that explain statistically significant amounts of variance in the output have been included in the model. This approach avoids having to treat all of the independent uncertain variables simultaneously in a single model.

The relative importance of the uncertain inputs is expressed in terms of the standardized regression coefficient (SRC). This is obtained by multiplying the value of the regression coefficient for a variable by its standard deviation and normalizing it by the standard deviation of the output. The larger the absolute value of the SRC, the more important is the contribution of the variable to the overall spread of the output. The SRCs can also be interpreted as regression coefficients that would be obtained from a regression analysis with the input and output variables normalized to zero mean and unit standard deviation. In general, the importance ranking deduced from the order of entry into the regression model is the same as that obtained from the absolute value of the SRC (or alternatively, from the absolute value of the rank correlation coefficient), especially if the input variables are uncorrelated or weakly correlated.

A more robust indicator of importance, particularly when the input variables are correlated, is the R^2-loss, which represents the reduction in the goodness-of-fit of the current regression model if the variable of concern is dropped from the regression model (RamaRao et al. 1998 [100487]). A large value of R^2-loss (i.e., a large decrease in explanatory power) indicates that the removed variable explained a large proportion of the variance in the output and, therefore, the variable is an important component of the model.

8.2.2 Entropy-Based Analyses

The information-theoretic concept of entropy is a useful metric for the characterization of uncertainty (or information) in the univariate case, and redundancy (or mutual information) in the multivariate case (Press et al. 1992 [103316]). Because mutual information is a natural measure of input variable relevance, it has been used as an indicator of variable importance in many areas of science such as language, speech and image processing, analyses of nonlinear systems, delay estimation in time series, neural network-based modeling and biomedical applications.

The following theoretical discussion is based on Press et al. (1992 [103316]). Let the input variable x and the output variable y have multiple possible states. For continuous variables, these could be taken as deciles (i.e., a total of ten states) or quintiles (i.e., a total of five states). This information can be compactly organized in terms of a contingency table–a table whose rows are labeled by the values of the independent variable, x, and whose columns are labeled by the values of the dependent variable, y. The entries of the contingency table are nonnegative integers giving the number of observed events for each combination of row and column.

The mutual entropy (information) between x and y, which measures the reduction in uncertainty of y due to knowledge of x (or vice versa), is defined as the difference between the sum of the individual entropies of x and y, and the joint entropy of x and y. Expressions for these entropies can be found in Press et al. (1992 [103316]), and involve simply counting the number of occurrences of various states of x alone, y alone and xy together.

Once the contingency table has been constructed, several measures of association can be calculated. One such useful measure is the R-statistic (Granger and Lin 1994 [159077]) which takes values in the range [0,1]. R is zero if x and y are independent, and is unity if there is an exact nonlinear relationship between x and y. It can also be shown that if x and y have a bivariate normal distribution, then the *R*-statistic is identical to the absolute value of the correlation coefficient between *x* and *y*.

The contingency table can also be visualized using a "bubble plot," where the entries of the contingency table are shown as bubbles of varying sizes. Here, the contingency table is organized such that the quintiles (or deciles) of the independent variable (input) increase from left to right, and that of the dependent variable (output) increase from top to bottom. The size of the bubble indicates how many observations fall in each quintile-quintile (or decile-decile) box.

The entropy-based measure *R*-statistic can thus be recognized as a very general tool for quantifying the strength of an association. It is applicable to both linear/nonlinear and monotonic/nonmonotonic relationships, whereas the regression-based measures discussed earlier are restricted to linear and monotonic associations only.

As an example, a bubble plot for an important variable identified on the basis of the *R*-statistic is presented in Figure 8.2.2-1. A V-shaped pattern is revealed in this figure, indicating that the highest quintile dose values correspond to those in the middle of the input distribution. This nonmonotonic association, although evident in a scatter plot (Figure 8.2.2-2), would have been difficult to identify using regression analyses because these are restricted to examining only monotonic relationships.

8.2.3 Classification-Tree-Based Analysis

Although regression modeling is routinely used for identifying key drivers of uncertainty for the entire output, specialized approaches may be required for examining small subsets (e.g., top and bottom deciles) of the output. To this end, classification tree analysis (Breiman et al. 1998 [151294]) can provide useful insights into what variable or variables are most important in determining whether outputs fall in one or the other (extreme) category. Traditional applications of classification trees have primarily been in the fields of medical decision making and data mining for social sciences.

A binary decision tree is at the heart of classification tree analysis. The decision tree is generated by recursively finding the variable splits that best separate the output into groups where a single category dominates. For each successive fork of the binary decision tree, the algorithm searches through the variables one by one to find the purest split within each variable. The splits are then compared among all the variables to find the best split for that fork. The process is repeated until all groups contain a single category (as far as practicable). In general, the variables that are chosen by the algorithm for the first several splits are most important, with less important variables involved in the splitting near the terminal end of the tree.

The tree-building methodology used in TSPA-SR and also planned for TSPA-LA is based on a probability model approach (Venables and Ripley 2001 [159088]). Classifiers at each node are selected based on an overall maximum reduction in deviance, for all possible binary splits over all the input variables. The classification tree is built by successively taking the maximum reduction in deviance over all the allowed splits of the leaves to determine the next split.

Termination occurs when the number of cases at a node drops below a set minimum, or when the maximum possible reduction in deviance for splitting a particular node drops below a set minimum.

The use of classification trees in sensitivity analysis involves several steps beyond the basic tree construction. After the tree is built, the nodes are evaluated as to their relative contribution in determining important variables. The earliest splits contribute most to the reduction in deviance and are considered to be most important in the classification process. The later splits may be marginally important, or may simply fall in the range of statistical “noise.” Usually, an attempt is made to “prune” the tree (i.e., reduce the number of splits) to the point where only a handful of variables are left which can be used to classify the majority of the outputs. Pruning is usually accomplished by increasing the minimum reduction in deviance necessary for node splitting and then rebuilding the tree.

If two or three variables are identified as holding most of the explanatory (or classification) power in the model, the results can be further visualized through the use of a partition plot. A partition plot is a scatter plot of the two most important input variables, with the categorical outcomes defined by unique symbols. One horizontal and one vertical line show the location of the splits for the input variables. The main utility of a partition plot is to display the clustering of outcomes (if any) in the parameter space. This helps provide a visual interpretation of the decision rules generated by the classification tree algorithm.

The binary classification tree approach outlined above (and the tree based model in general) has several advantages when compared to linear and additive models:

- Tree-based models are adept at capturing non-additive behavior. Because the output from TSPA-LA analyses come from complex nonlinear models of physical processes, not being restricted to simple additive input-output models is a distinct advantage over conventional linear regression based sensitivity analyses.
- Tree-based models can handle more general (i.e., other than of a particular multiplicative form) interactions between predictor variables.
- Tree-based models are invariant to monotonic transformations of the input variables.

As an example, a classification tree is presented in Figure 8.2.3-1, where only four variables are needed to perfectly categorize the model outcomes into high and low groups (i.e., dose in the top and bottom 10 percentiles). A visual interpretation of the key decision rules generated by the classification tree algorithm is provided by the partition plot shown in Figure 8.2.3-2. High values for both variables leads to high doses, and conversely, low values for at least one of these two variables leads to low doses. Such insight about the interaction of two important variables and how they affect the model outcome is typically missing from standard input-output scatter plots or tables of regression analysis results.

8.2.4 Implementation Issues

Regression-based measures of uncertainty importance are well-known in the sensitivity analysis literature. However, the applicability of these techniques is restricted to conditions where nonmonotonic patterns and possible variable interactions do not influence the input-output relationship. Entropy-based measures, on the other hand, have a broader applicability for identifying significant input-output patterns, monotonic or otherwise.

Classification trees are a useful tool for identifying key variables affecting extreme outcomes in probabilistic model results. When supplemented with a two-variable decision tree and/or a partition plot, the separation of extreme outcomes in the uncertain parameter space is easy to visualize and explain. The power of classification trees lies in handling nonlinear and non-additive behavior, albeit for monotonic input-output models.

The methods discussed in this section are limited to those that utilize only the sampled input values and computed model outcomes from a Monte Carlo simulation experiment, and do not require new simulations. However, if additional model calculations do not entail significant computational expense, then two other uncertainty importance analysis techniques may be utilized. The Morris method (Morris 1991 [159078]) uses an efficient sampling scheme to evaluate the sensitivity of model output to an uncertain input at various points in the parameter space and rank the variables accordingly. In the Fourier Amplitude Sensitivity Test, or FAST (Saltelli et al. 1999 [159079]), the overall variance is decomposed into terms representing first-order (individual variable) and higher-order (variable interaction) contributions as the basis for importance ranking.

Finally, it should be noted that there is no single “perfect” technique for uncertainty importance analyses. One or more techniques may be necessary, and/or appropriate, depending on the nature of input-output relationship. To that end, the following step-wise procedure will be utilized in TSPA-LA:

- Carry out stepwise linear rank regression analysis to identify key contributors to output variance.
- Check for significant nonmonotonic input-output patterns using entropy analysis.
- Use classification tree analysis to determine how key variables affect extreme model outcomes.

8.3 APPROACH TO SUPPORT THE MULTIPLE BARRIER ANALYSES

The discussion of the TSPA-LA analyses so far has concentrated on the demonstration of compliance with the individual protection performance objective at 10 CFR 63.113(b). In addition, this discussion has addressed the analyses to be conducted for the groundwater protection objective at 10 CFR 63.113(c). What has not been discussed so far is the role these TSPA-LA analyses will play in supporting the multiple barrier requirements at 10 CFR 63.115. These requirements call for DOE to:

- Identify those design features of the engineered barrier system and natural features of the geologic system that are considered barriers important to waste isolation
- Describe the capability of the barriers, identified as important to waste isolation, to isolate waste, taking into account uncertainties in characterizing and modeling the behavior of the barriers.
- Provide the technical basis for the description of the capability of the barriers, identified as important to waste isolation, to isolate waste. The technical basis for each barrier's capability shall be based on and consistent wit the technical basis for the performance assessments used to demonstrate compliance with 10 CFR 63.113(b) and (c).

Each of these requirements is discussed in the following.

8.3.1 Description of Barriers

The definitions in 10 CFR 63.2 clarify the requirement to identify the barriers considered important to waste isolation. The term "barrier" means "any material, structure or feature that prevents or substantially reduces the rate of movement of water or radionuclides from a proposed repository to the accessible environment, or prevents the release of or substantially reduces the release rate of radionuclides from the waste". Further, 10 CFR 63.2 defines "barrier important to waste isolation" as "those natural and engineered barriers whose function is to provide a reasonable expectation that high-level waste can be disposed of without exceeding the requirements of 10 CFR 63.113(a) and (b). "

The barriers important to waste isolation at Yucca Mountain are broadly categorized as natural barriers (associated with the geologic and hydrologic setting) and engineered barriers. The engineered barriers complement the natural barriers by prolonging the containment of radionuclides within the repository and limiting their eventual release.

The natural barriers important to waste isolation consist of the following:

- Surficial soils and topography, which limit water infiltration
- Unsaturated zone rock units above the repository horizon, which limit water flux into repository drifts
- Unsaturated zone rock units below the repository horizon, which limit radionuclide transport
- Volcanic tuffs and alluvial deposits below the water table, which limit radionuclide transport in the saturated zone.

The engineered barriers important to waste isolation consist of the following:

- The drip shield, which protects the waste package from rock fall and limits the water contacting the waste package and water available for advective transport through the waste package and the invert

- The waste package, which limits the water contacting the waste form
- Cladding on spent fuel, which limits the water contacting the CSNF portion of the waste form
- The waste form that limits the rate of release of radionuclides to the water that contacts the waste
- The drift invert which limits the rate of release of radionuclides to the natural barriers.

8.3.2 Description of Barrier Capability

The complete description of the capabilities of barriers important to waste isolation will focus on the capabilities of these barriers to limit movement of water or radionuclides. This description will include model and parameter uncertainties in the discussion of the capability to limit movement of water or radionuclides. It will discuss the changes in barrier capability over the 10,000 year compliance period and the effects of spatial variability in preventing or substantially delaying movement of water or radionuclides. This approach addresses KTI agreements TSPAI 1.01, and TSPAI 1.02.

The level of information provided in the description of barrier capabilities will be commensurate with the relative importance of these barriers in meeting the individual protection requirement of 10 CFR 63.113(b). Accordingly, this description will relate the capabilities of the barriers to limit the movement of water or radionuclides to the TSPA analyses to address individual protection. For the most part, this discussion will be based on the physical arguments that underlie the TSPA results. In addition, the description will include, as appropriate, quantitative analyses that include: (1) intermediate performance analyses, and (2) pinch-point analyses. The pinch-point analyses are a specific form of the intermediate performance analyses, with the only metrics of interest being those related to the reduction in mass at several discrete locations. The intermediate performance analyses, as proposed, are more general and include model subcomponent characteristics as performance measures.

Intermediate Performance Analyses-This approach to evaluating the contribution that different barriers provide to the overall performance of the repository system involves analyzing the intermediate performance of the total system as the system evolves over time. Here, intermediate performance refers to the functioning of individual subcomponents of the TSPA-LA model, rather than on the behavior of the entire waste disposal system. This approach describes the results of the system’s temporal and spatial evolution and the uncertainty in this evolution. Thus, the intermediate performance analyses involve examining the internal workings of the reference case simulation for the nominal scenario class. Performance measures of interest include such characteristics of the TSPA-LA model as percolation flux, seepage percentage as a function of percolation flux, time to first breach of drip shield and waste package, fraction of fuel intact, groundwater breakthrough times, etc. Examining the intermediate results provides insight into how different components contribute to total system performance. These results, which will be derived directly from the TSPA-LA model (and not from any “extreme scenario” or “degraded barrier” simulation), will enable uncertainty in barrier characteristics and barrier interdependence to be taken into account. The intermediate performance analyses as described here build upon the type of subsystem analyses discussed in detail for the nominal scenario class in Section 8.1.1.

Pinch-Point Analyses-The pinch-point analysis approach is based on the processing of output from TSPA calculations at subsystem boundaries, or "pinch-points". These are locations where mass or energy is being transferred from one modeling domain (or subsystem or barrier) to another. Because the engineered and natural barriers seek to isolate waste from the environment by attenuating the movement of radionuclides, thus reducing the amount of mass released, two metrics related to the reduction in mass are proposed to measure the effectiveness of different barriers for waste isolation. These barrier effectiveness measures provide an indication of how the contaminants are distributed throughout the system, as well as an understanding of how the barriers are acting together to provide waste isolation.

The first metric quantifies the absolute mass reduction within each barrier (i.e., how much mass is retained in each barrier as a fraction of the initial inventory). Figure 8.3.2-1 provides a visual assessment of such a metric for a single nuclide, technetium-99, in an evaluation of the Canadian repository program (Goodwin et al. 1994 [124152], Figure 6-7). Figure 8.3.2-1 shows how technetium-99 is retained within different barriers and isolated from the biosphere at two different points in time: 10,000 years and 100,000 years. However, this definition of barrier effectiveness factor tends to understate the importance of downstream barriers, which receive a small fraction of the initial inventory. Therefore, a second barrier effectiveness factor is proposed to quantify the relative mass reduction in each barrier. Here the inflowing mass for the barrier is used as the normalizing factor (for the amount of mass retained within the barrier) as opposed to the initial inventory.

As described above, the pinch point analyses can help quantify the capabilities of barriers to radionuclide transport. Capabilities of barriers to restrict water movement (i.e., those above the repository) can be made in terms of average flux across the repository or on a per-package basis, (i.e., how the precipitation flux gets transformed into a smaller quantity contacting the packages).

8.3.3 Technical Basis for Describing Barrier Capability

The technical basis for the description of the capabilities of the barriers important to waste isolation is required to be consistent with the technical basis for the performance assessments used to demonstrate compliance with 10 CFR 63.113(b) and (c). As planned for TSPA-LA, in all cases, the technical basis for both the TSPA-LA model and the multiple barrier analysis will be the same set of AMRs. This will be the case regardless of whether the description of barrier capabilities is based on physical arguments (where the conceptual basis for TSPA-LA models and multiple barrier analysis will be consistent), or intermediate performance and pinch-point analysis (where the mathematical basis for TSPA-LA models and multiple barrier analysis will be consistent). In this sense, the technical basis for the multiple barrier analysis will not only be consistent with the performance assessments, it will be the same.

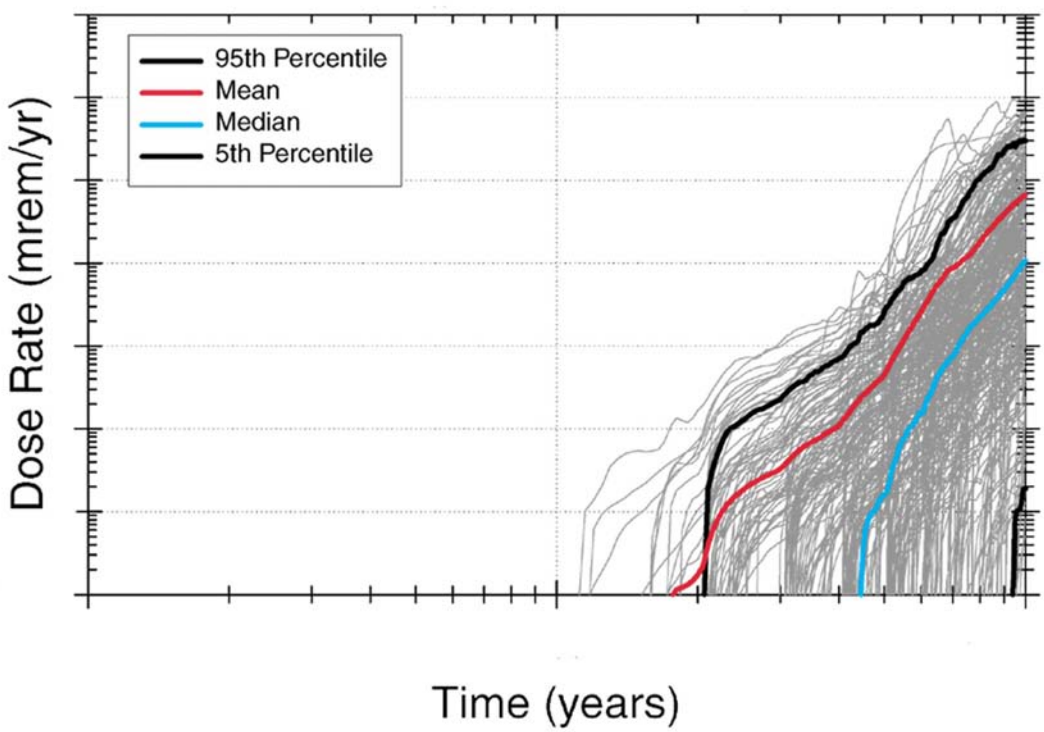


Figure 8.1.1-1. Example of an Expected Dose Time History, along with Running 5th, 50th and 95th Percentile Curves

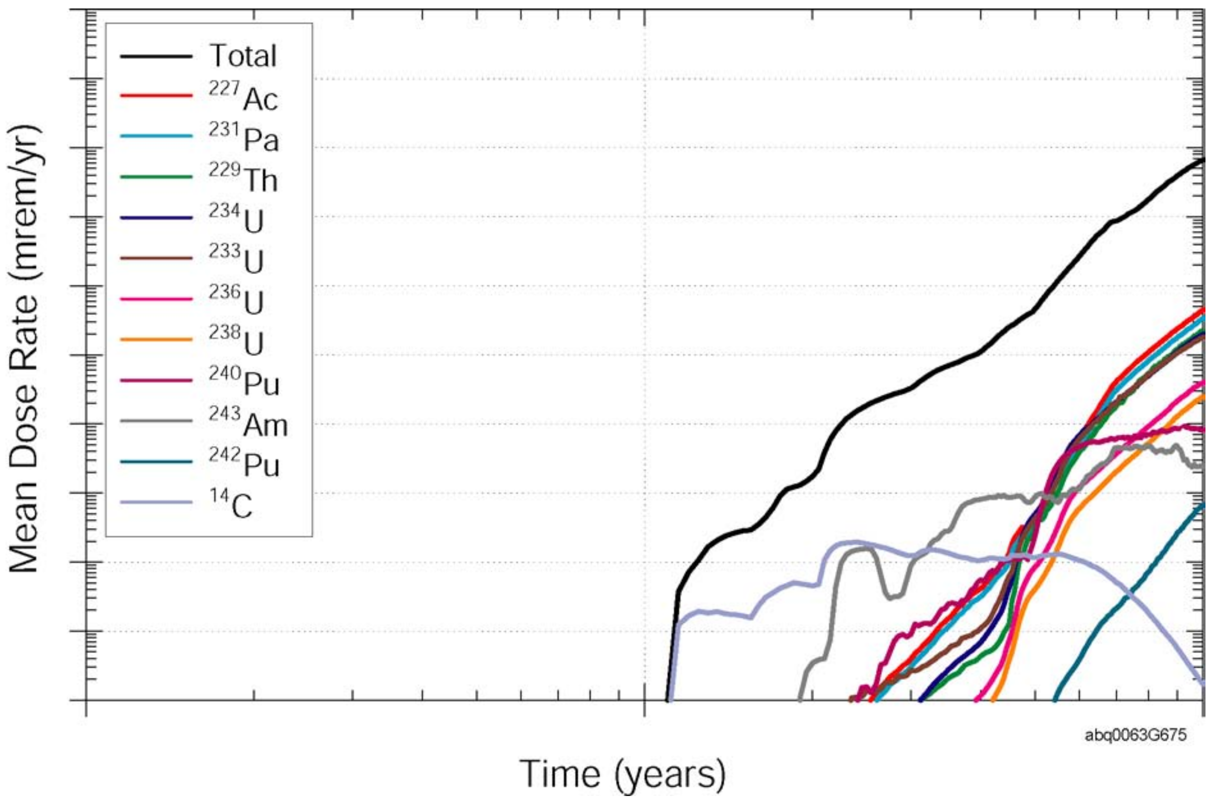


Figure 8.1.1-2. Example of Key Radionuclides and their Contributions to Expected Dose

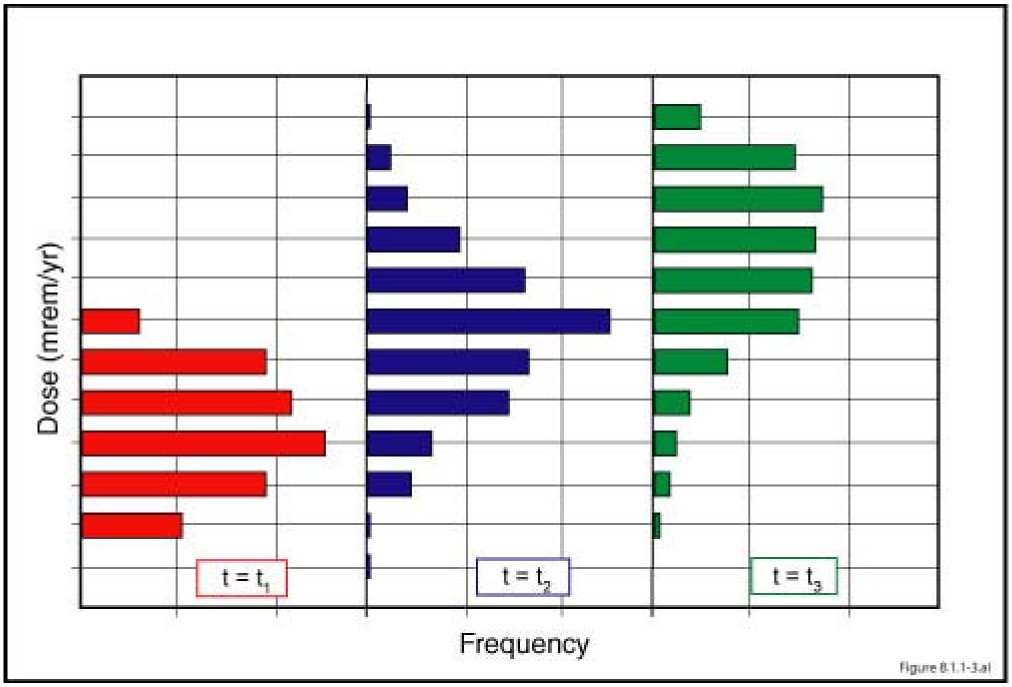


Figure 8.1.1-3. Example of Side-by-Side Histogram of Dose at Selected Times

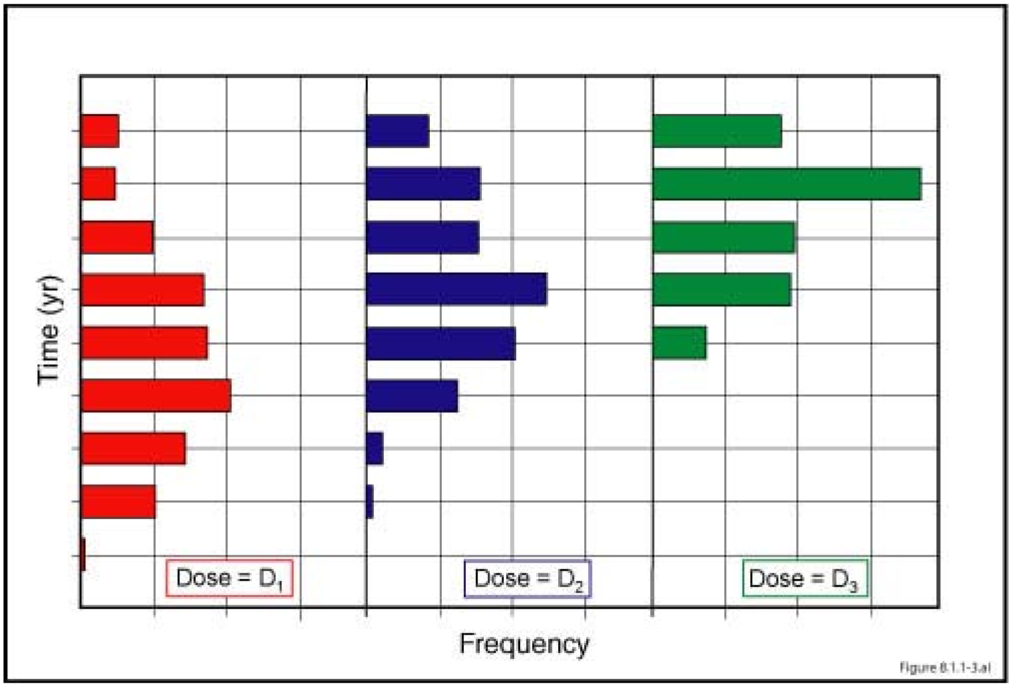


Figure 8.1.1-4. Example of Side-by-Side Histogram of Time to Reach Specified Dose

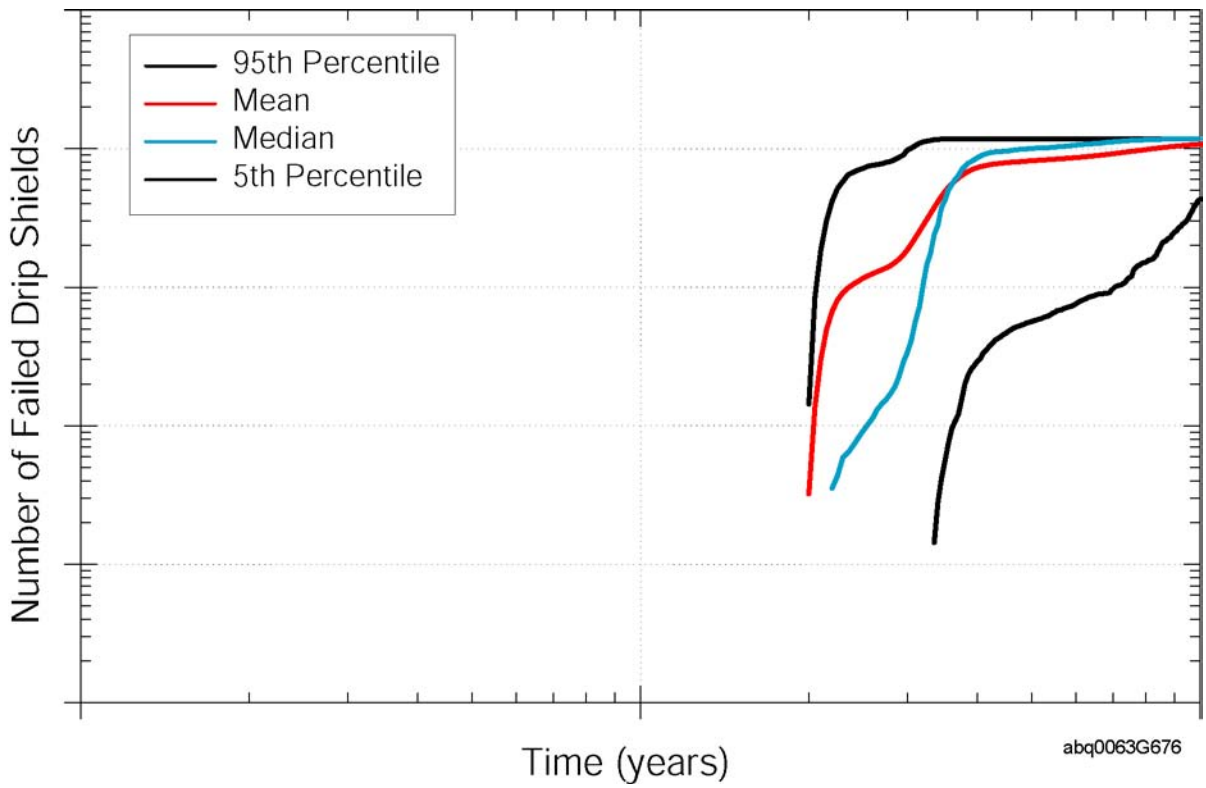


Figure 8.1.1-5. Example of Cumulative Drip Shield Failures

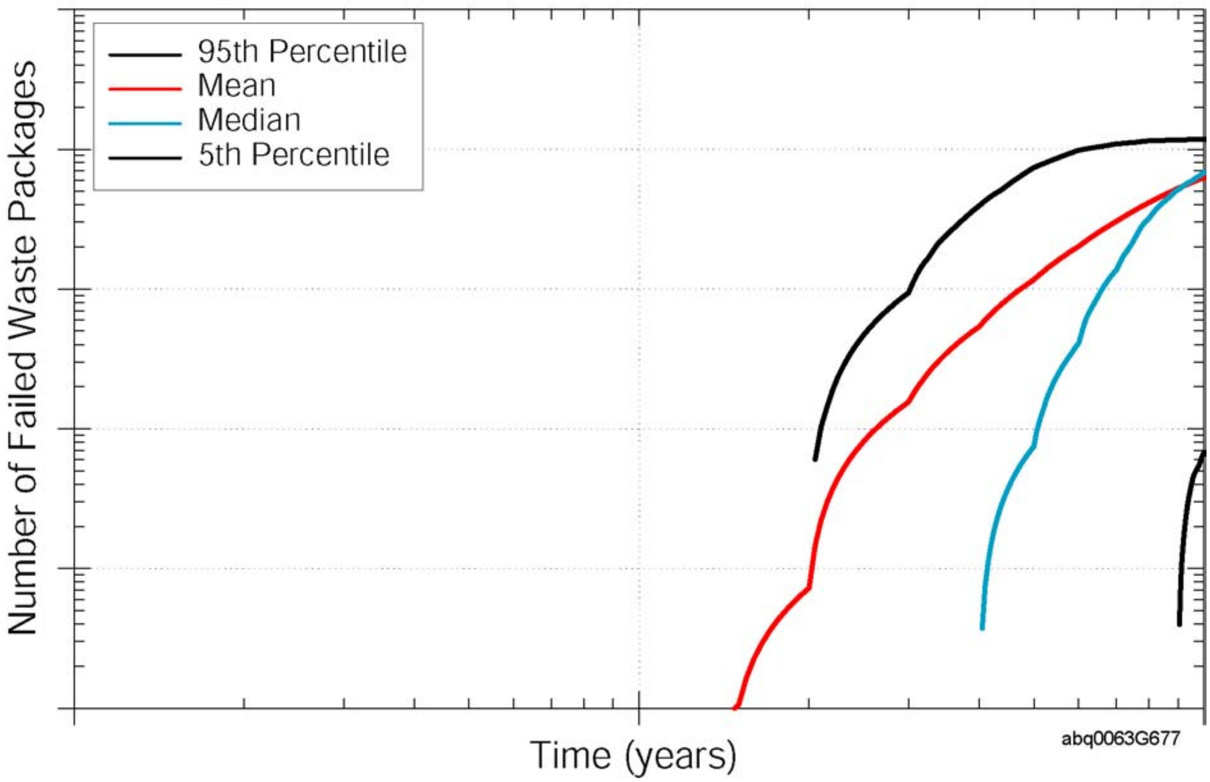


Figure 8.1.1-6. Example of Cumulative Waste Package Failures

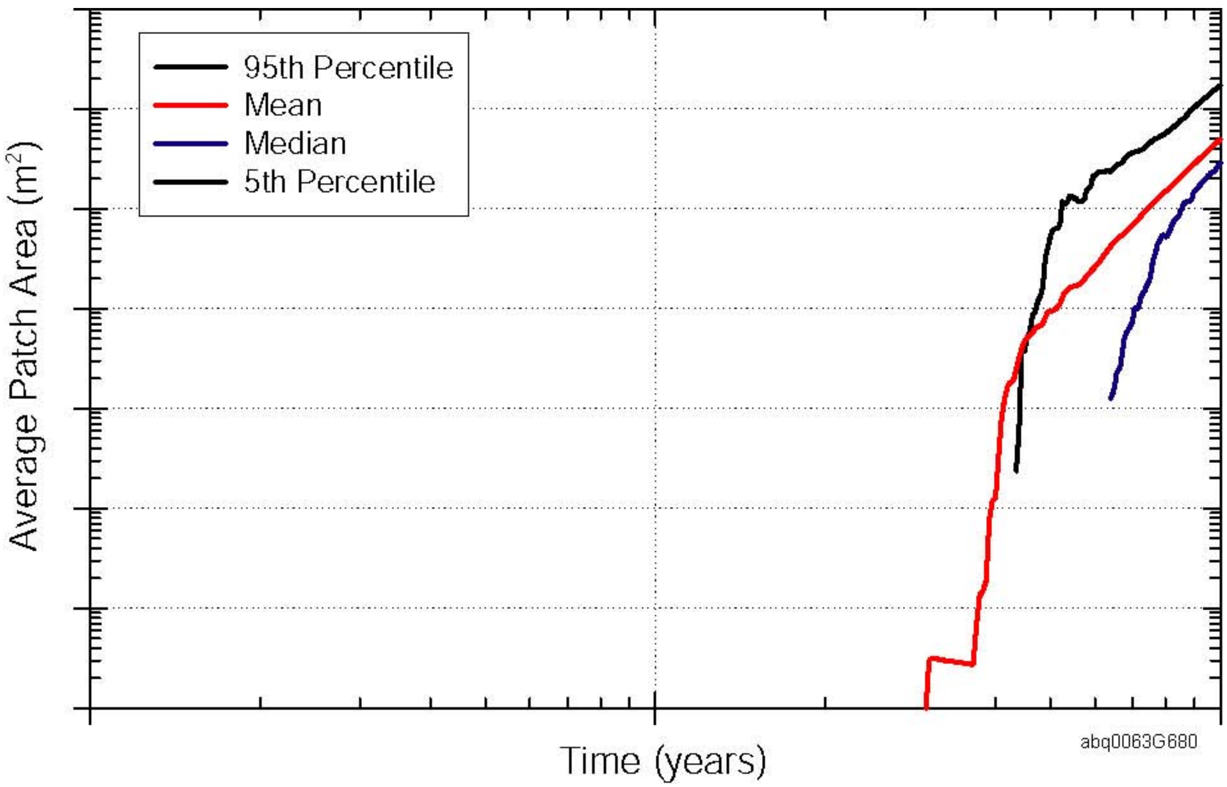


Figure 8.1.1-7. Example of Waste Package Opening Area

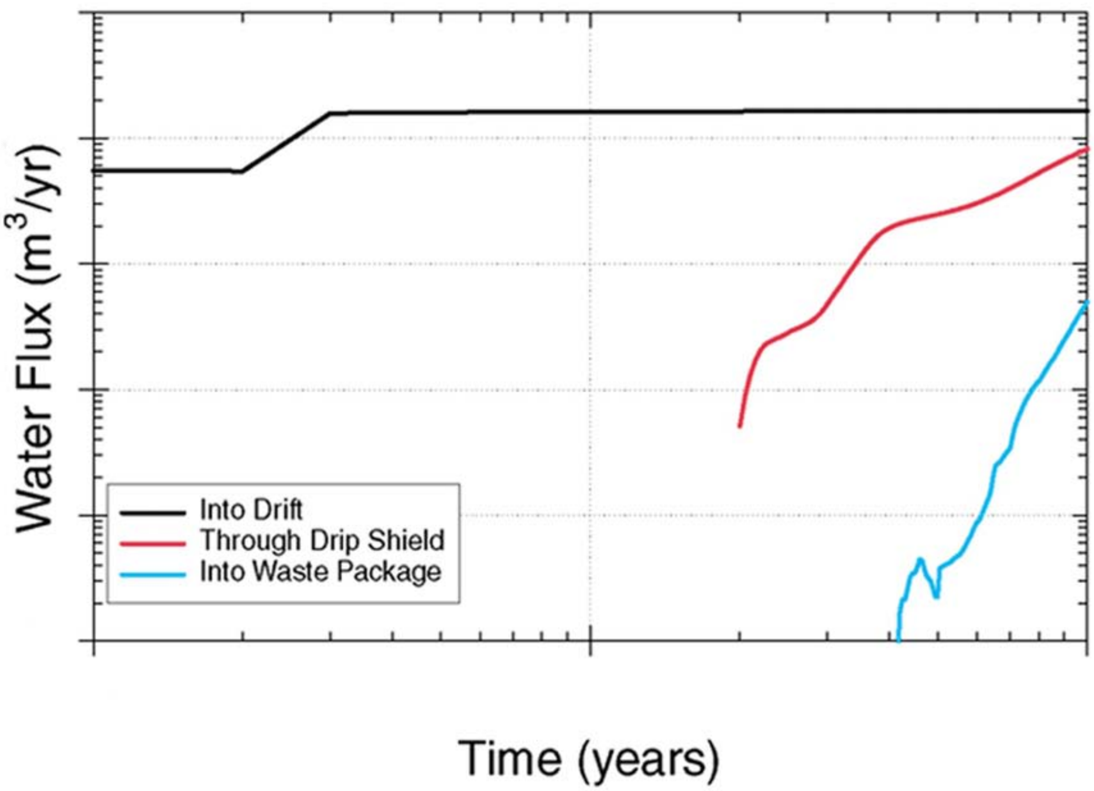


Figure 8.1.1-8. Example of Water Flow Rates into Drift, Through the Drip Shield and into Waste Package

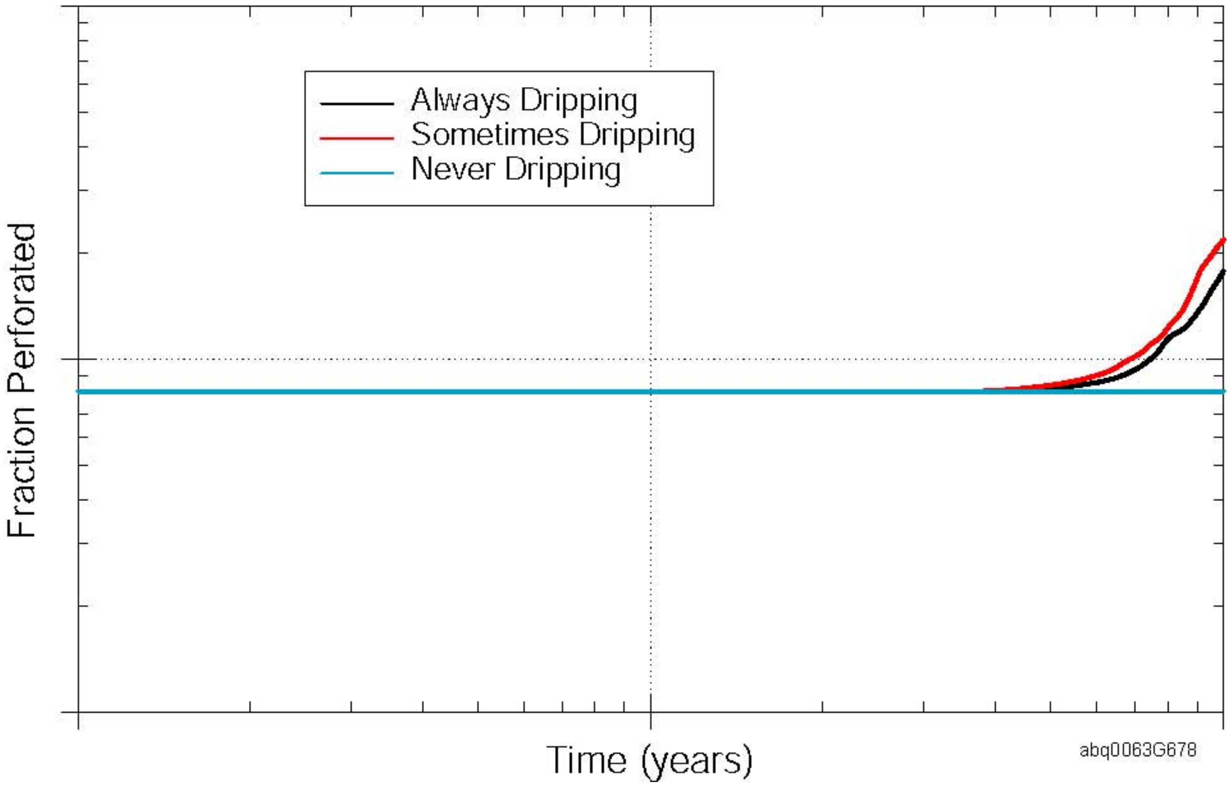


Figure 8.1.1-9. Example of Fractional Cladding Failures

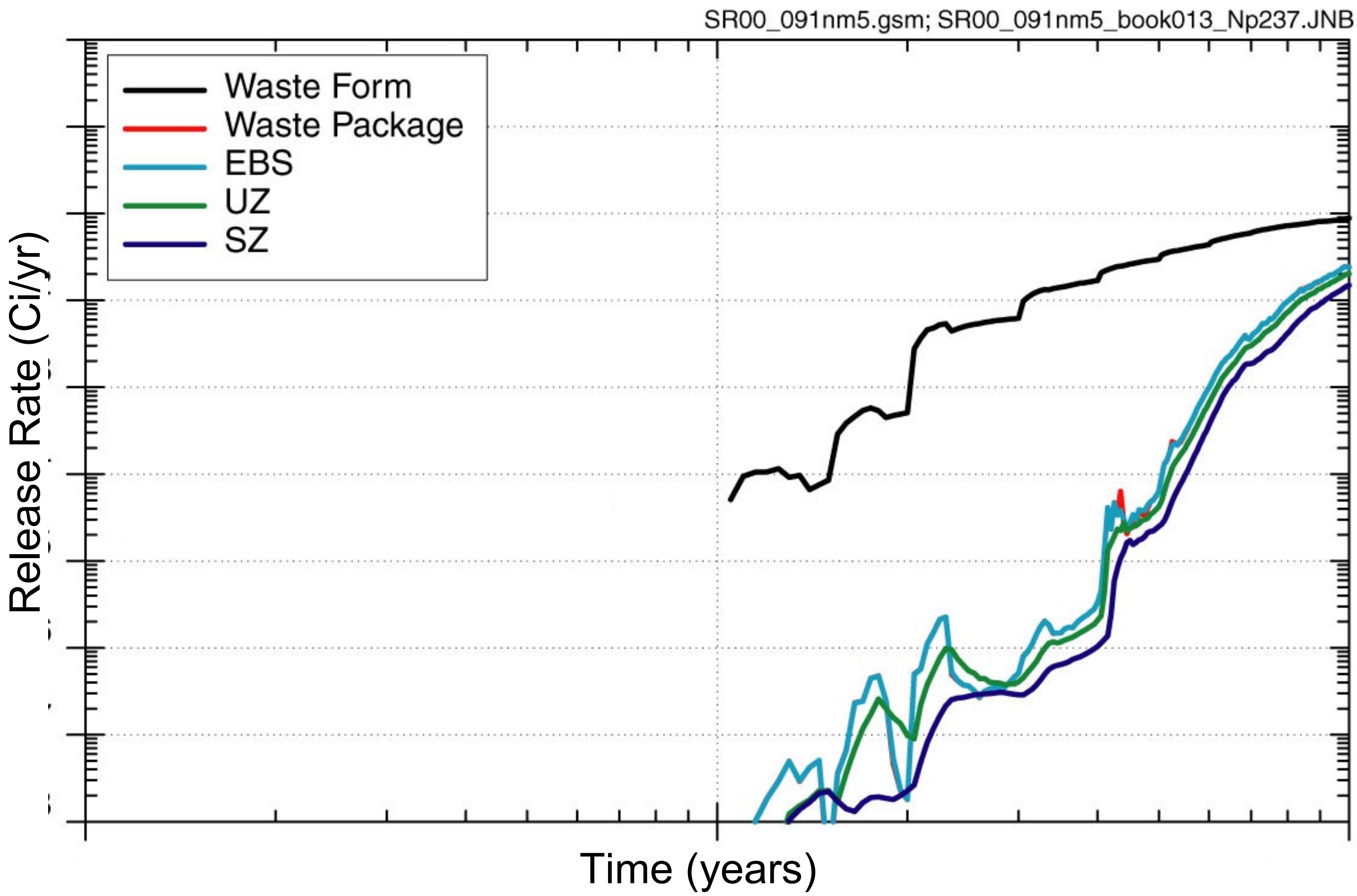


Figure 8.1.1-10. Example of Mean Release Rates for a Key Radionuclide

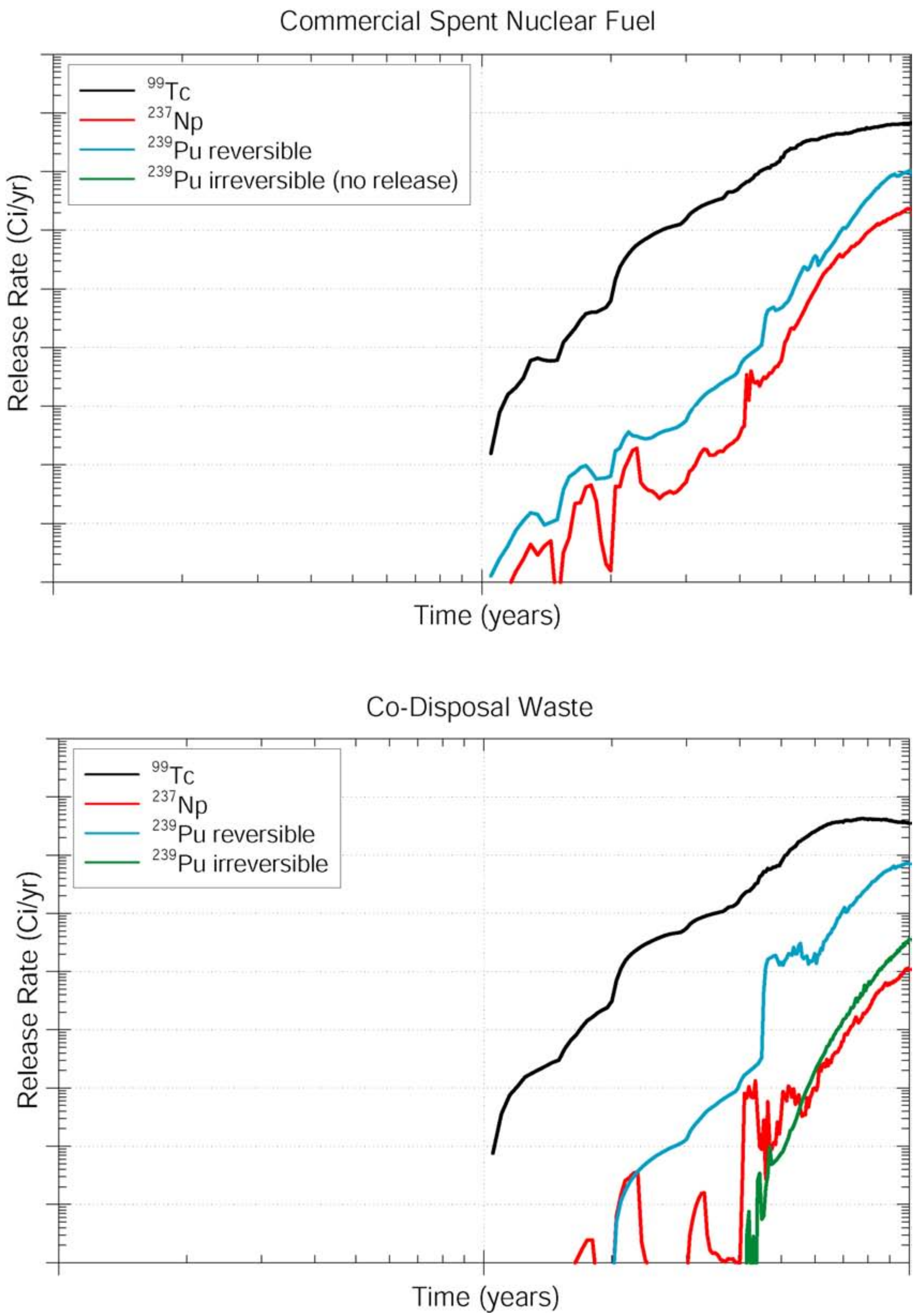


Figure 8.1.1-11. Example of EBS Release Rates from Different Waste Types

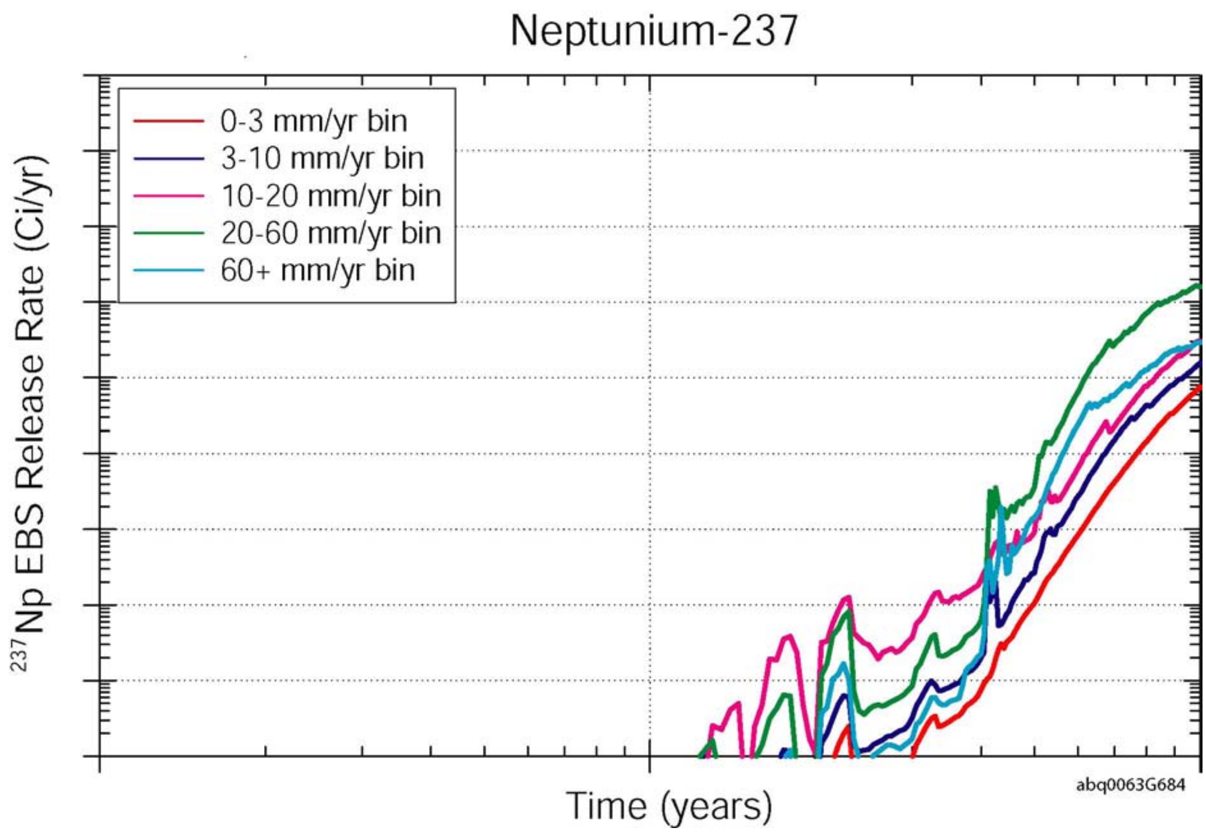


Figure 8.1.1-12. Example of UZ Release from Different Infiltration Bins

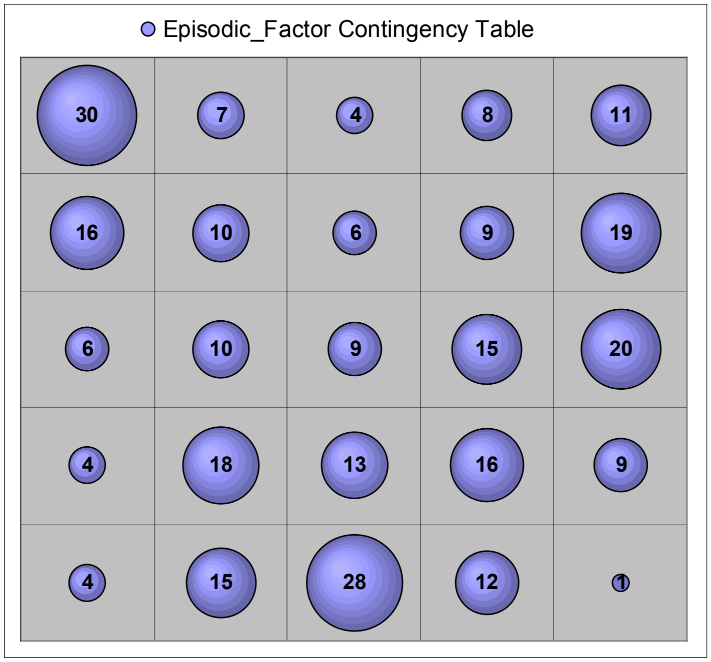


Figure 8.2.2-1. Example Bubble Plot Showing Episodic Factor Quintiles (x-axis) vs Dose Quintiles (y-axis)

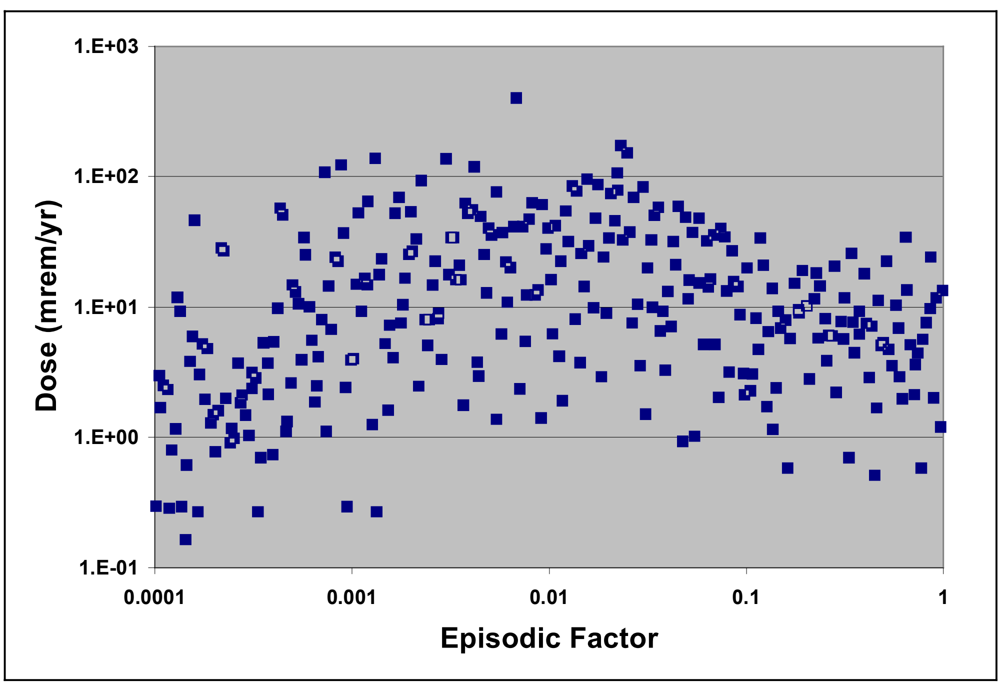


Figure 8.2.2-2. Example Scatter Plot for Two Variables

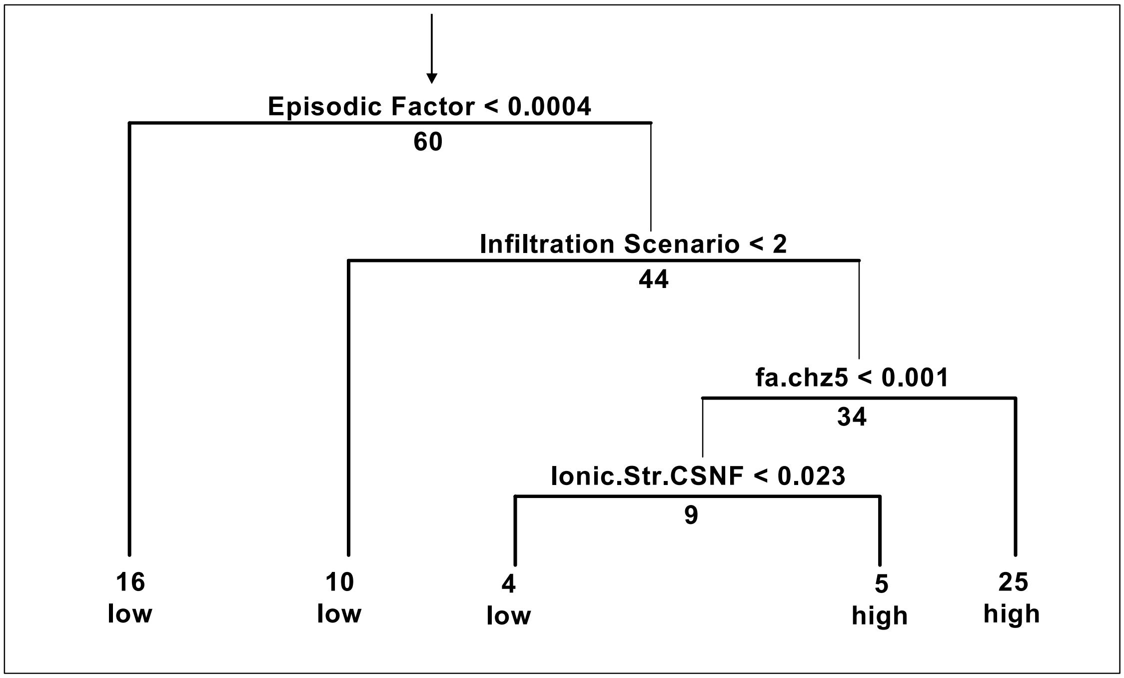


Figure 8.2.3-1. Example Classification Tree Showing Decision Rules for Separating High-dose and Low-dose Producing Realizations

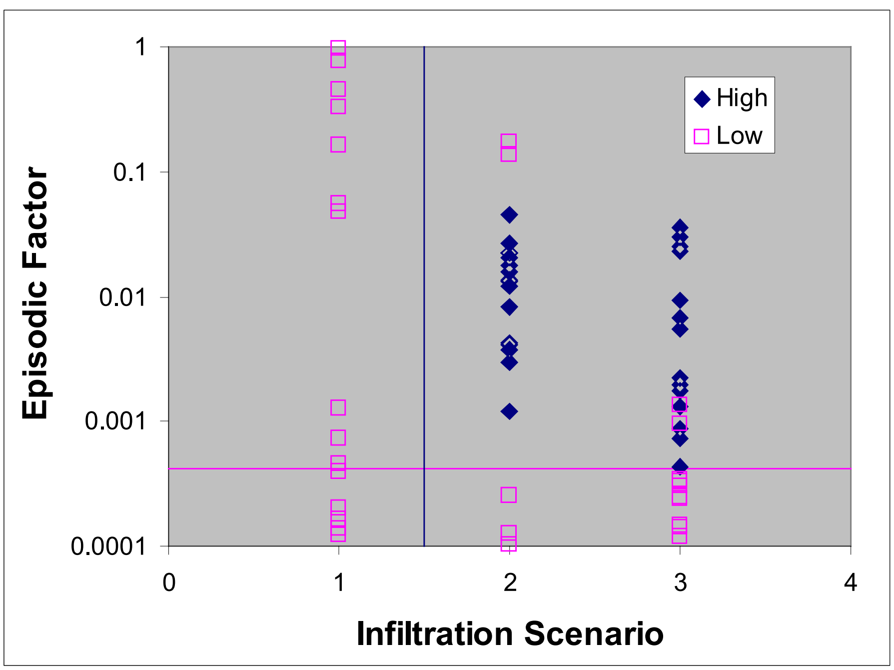
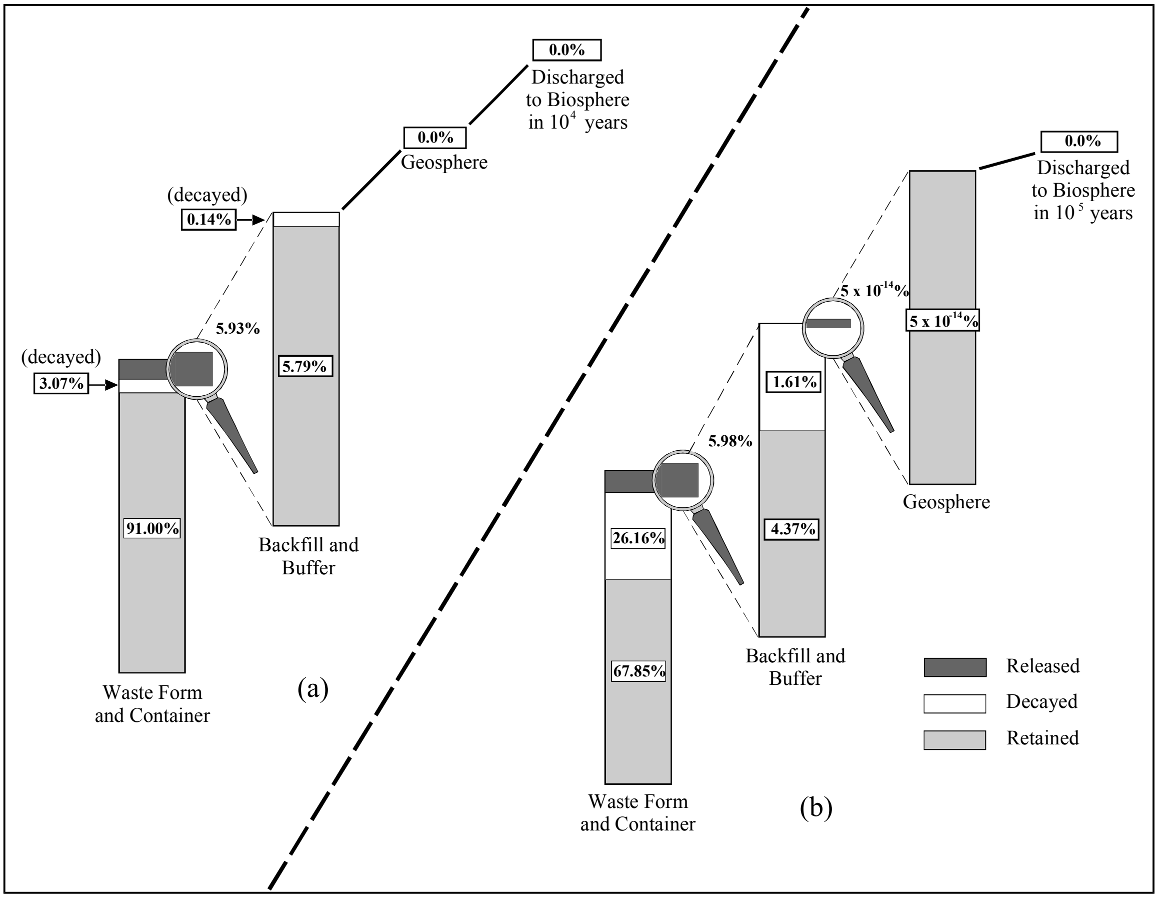


Figure 8.2.3-2. Example Partition Plot Showing Clustering of High- and Low-Outcomes in the Parameter Space of the Two Most Important Variables



Source: Goodwin et al. 1994 [124152], Figure 6-7

Figure 8.3.2-1. Graphical Depiction of Barrier Effectiveness Showing Distribution of Tc-99 in the Disposal System after (a) 10,000 Years and (b) 100,000 Years

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9. SUMMARY

The TSPA-LA methods and approach are based on NRC requirements and Office of Civilian Radioactive Waste Management (OCWRM) project Administrative Procedures. A brief summary of the approach, traceability, transparency, and analyses used to satisfy the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria follows.

9.1 SUMMARY OF APPROACH

The approach to be used for development, control, analysis and documentation of the TSPA-LA model is similar to what has been done for previous TSPA iterations. Of increased importance for TSPA-LA, compared to other TSPAs, is the need to meet the requirements of 10 CFR Part 63, and the acceptance criteria of the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]), and to maintain appropriate configuration control over the information, software, models, and documentation. Processes and procedures are in place within the TSPA Department as well as in the supplying organizations, for the appropriate configuration control.

The process for developing inputs (parameters, abstractions, alternative conceptual models, and uncertainty) for the TSPA is integrated across the Performance Assessment Project, as well as with other suppliers (e.g., National Spent Nuclear Fuel Program, Naval Reactors). This effort will provide for consistent, defensible inputs to the TSPA-LA model. Also, the process will follow the enhanced FEPs development approach to develop the FEPs ultimately utilized in the TSPA. Scenario development has led to the definition of two scenario classes: nominal scenario class, and disruptive event scenario class. The disruptive event igneous scenario class will have two modeling cases: volcanic eruption modeling case, and igneous intrusive modeling case. The disruptive event seismic scenario class will be a class by itself. The stylized human intrusion analysis will be treated separately from the scenario classes, primarily because the event as defined in 10 CFR Part 63.321 is not expected to occur in the regulatory time period (10,000 years).

The probabilistic simulations of the total system will be evaluated to determine the key factors contributing to the dose at 18 km. Current plans are to analyze simulations up to 20,000 years, and to utilize 300 realizations per analysis. These plans may be modified for various reasons as the analyses progress.

The documentation suite for the TSPA-LA will include the TSPA-LA Model Document, the TSPA-LA Analysis Document, and the corresponding sections in the LA itself. The latter may be simply extracts or simple syntheses of the foundation TSPA-LA documents. In addition, a large volume of supporting documents will be directly referenced from the TSPA-LA documents including model reports, analysis reports, design documents, and calculation documents (see Appendix G for planned document hierarchy).

9.2 SUMMARY OF TRANSPARENCY AND TRACEABILITY

An overall objective of any integrated performance assessment, but in particular total system performance assessments of proposed nuclear waste repositories, is to provide a "transparent and traceable" analysis that allows the reader the opportunity to understand the basic assumptions and their scientific basis in such a way that he or she may understand and test the accuracy and reproducibility of the conclusions. AP-SIII.10Q, *Models*, has defined transparency as the attribute of producing documents that are sufficiently detailed as to purpose, method, assumptions, inputs, conclusions, references, and units, such that a person technically qualified in the subject can understand the documents and ensure their adequacy without recourse to the originator. AP-SIII.10Q, *Models*, has defined traceability as the ability to trace the history, application, or location of an item, data, or sample using recorded documentation.

Throughout the TSPA-LA documentation, the underlying data, assumptions, models, and analyses will be discussed with appropriate conceptual drawings and integration graphics to illustrate the role of the model component, the technical basis of the model component, and the information flow from or to each model component. In addition, interim results will be presented both at the TSPA system level and the subsystem level to illustrate how information (in terms of mass, water, energy, activity) flows from one part of the system to the next in the integrated total system model. Also, the hierarchy of all analysis and model reports that support the final information feed to the TSPA-LA model will be presented.

The defensibility of the analyses and models that support the TSPA-LA model is contained in the relevant AMRs. It is the AMRs that provide the fundamental scientific underpinning, and the associated assumptions and conservatisms necessary for a defensible, yet reasonably cautious analysis of expected performance.

It is beyond the scope of the TSPA documentation to summarize the depth and breadth of the information contained in the analysis model reports that form the basis for the TSPA-LA. The individual models are based on appropriate site-specific information, analog data, and relevant literature data sources that have been integrated by the principal scientific investigators to provide a reasonable and defensible characterization of each individual process relevant to postclosure performance. Quantifiable uncertainty in the individual model component was also included as appropriate.

In addition to the analysis and model reports providing a traceable chain of references for the defensibility of the scientific bases for the TSPA-LA, they will also provide a hierarchy of data tracking numbers. The sources and hierarchy of data sets used as input to the TSPA-LA model will be summarized in the TSPA-LA Analysis Document, with additional detail in the TSPA-LA Model Document. The status of each data set used as input to the TSPA-LA model can be ascertained by tracing the data set and all its predecessors using the TDMS and DIRS databases. This capability allows the DOE and NRC to track the status of all data sets used in the development of the postclosure safety case.

The data, analyses, and models used as the technical basis for the TSPA-LA, as well as the assumptions, uncertainty, and variability that go along with these data, analyses, and models will be traceable back to their source documents and data sets. This traceability allows all interested reviewers to examine the defensibility of the individual model components and reach their own conclusions regarding their scientific adequacy.

9.3 SUMMARY OF UNCERTAINTY TREATMENT IN TSPA-LA ANALYSES

TSPAs are, by their very nature, uncertain projections of the possible behavior of the individual model components describing the relevant processes affecting the containment and isolation of radioactive wastes from the biosphere. This uncertainty is explicitly included in the models and resulting analyses in the form of discrete probability distributions that encompass the range of possible outcomes.

There remains uncertainty in the individual process models and their abstraction into the TSPA-LA model. Much of this uncertainty will be quantified and included in the TSPA-LA model. The TSPA-LA results will reflect this quantified uncertainty.

In addition to the quantified uncertainty in the TSPA-LA model, there may also be unquantified uncertainty that will be represented by using an appropriately realistic representation of a particular model. These representations (which may be necessarily conservative) result when there is insufficient information available or significant complexity exists that is not amenable to quantified uncertainty. Elicitation approaches could be used if it was desired to quantify the uncertainty in these conservative judgments.

9.4 SUMMARY OF HOW THE APPROACH SATISFIES YUCCA MOUNTAIN REVIEW PLAN ACCEPTANCE CRITERIA

The methods and approach presented in this document for the TSPA-LA will develop a TSPA-LA model and analyses that will satisfy the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria for postclosure repository safety. The *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) requires that the NRC review the barriers important to waste isolation. The TSPA-LA approach to the multiple barrier analysis was briefly described in Section 8.3. The intent is to briefly describe the barriers, and provide some evaluation of their capabilities as to their effect on water and radionuclide movement from the repository.

The scenario analysis approach is another significant part of the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria. Both nominal and disruptive scenario classes have been defined, and will be analyzed in the TSPA-LA. The approach to this selection of scenarios has been discussed, along with the approach to ensure appropriate identification and screening of the FEPs relevant to the Yucca Mountain site. The FEPs, as well as the concomitant parameters, abstractions, alternative conceptual models, and associated uncertainty, will be defined and developed utilizing the new integrated approach discussed in Section 3. This approach brings together the necessary SMEs and TSPA personnel to develop consistent, traceable inputs for the TSPA-LA model.

The *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) requires traceability of the inputs to the TSPA-LA. The controls of the process of testing, developing, and analyzing the TSPA-LA model that contribute to the overall traceability of the analyses are described in Section 6.

Detailed consideration of all *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria has been incorporated into the planning of the TSPA-LA, including the supporting PA and Design organizations. This effort is designed to lead to an integrated safety assessment of the repository, that is defensible, traceable, and readily transparent to the technical reviewers of the analysis.

10. REFERENCES

The following is a list of the references cited in this document, Column 1 represents the unique six digit DIRS number, which is placed in the text following the callout (e.g., (BSC 2001 [154659])). The purpose of these numbers is to assist the reader in locating a specific reference. The reference list is ordered numerically by the DIRS number.

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10.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

101680 64 FR 8640. Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, Nevada. Proposed rule 10 CFR Part 63. Readily available.

105725 ASTM C 1174-97. 1998. *Standard Practice for Prediction of the Long-Term Behavior of Materials, Including Waste Forms, Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 246015. ASTM C1174-97.

136421 AP-SIII.2Q, Rev. 0, ICN 2. *Qualification of Unqualified Data and the Documentation of Rationale for Accepted Data.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19991214.0625.

153202 AP-SV.1Q, Rev. 0, ICN 2. Control of the Electronic Management of Information. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000831.0065.

153493 AP-SIII.1Q, Rev. 0, ICN 1. *Scientific Notebooks.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000516.0002.

154534 AP-2.21Q, Rev. 1, ICN 0, BSCN 001. Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20010212.0018.

155216 66 FR 32074. 40 CFR Part 197, Public Health and Environmental Radiation Protection Standards for Yucca Mountain, NV; Final Rule. Readily available.

156605 10 CFR 63. Energy: Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada. Readily available.

156671 66 FR 55732. Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, NV. Final Rule 10 CFR Part 63. Readily available.

157282 AP-3.15Q, Rev. 3, ICN 1. *Managing Technical Product Inputs.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020102.0204.

158907 AP-SI.1Q, Rev. 3, ICN 4. Software Management. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020520.0283.

158908 AP-SIII.10Q, Rev. 0, ICN 2. Models. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020506.0911.

158987 AP-SIII.9Q, Rev. 0, ICN 1. Scientific Analyses. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020404.0083.

159044 AP-2.14Q, Rev. 2, ICN 1. Review of Technical Products and Data. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020701.0183.

159045 AP-3.11Q, Rev. 3, ICN 2. *Technical Reports.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020701.0189.

159254 AP-15.3Q, Rev. 0, ICN 0. Control of Technical Product Errors. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020212.0254.

159255 AP-SIII.3Q, Rev. 1, ICN 2. Submittal and Incorporation of Data to the Technical Data Management System. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020701.0177.

159475 DOE (U.S. Department of Energy) 2002. *Quality Assurance Requirements and Description.* DOE/RW-0333P, Rev. 12. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020819.0387.

159604 AP-2.27Q, Rev 0, ICN 0. *Planning For Science Activities.* Washington, DC: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020701.0184.

159727 AP-ENG-004, Rev. 1, ICN 0. *Resolution of Differing Professional Opinion.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020516.0093

APPENDIX A

ACRONYMS

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APPENDIX A ACRONYMS

ACM	alternative conceptual model
AECL	Atomic Energy of Canada, Ltd
AMR	analysis model report
AP	Administrative Procedure
ATL	Abstraction Team Lead
BDCF	biosphere dose conversion factor
BIO	biosphere
BSC	Bechtel SAIC Company, LLC
BTC	break-through curve
CDF	cumulative distribution function
CFR	Code of Federal Regulations
CNWRA	Center for Nuclear Waste Regulatory Analyses
CRWMS	Civilian Radioactive Waste Management System
CSNF	commercial spent nuclear fuel
DE	disruptive events
DIRS	Document Input Reference System
DLL	dynamically linked library
DOE	U.S. Department of Energy
DSNF	DOE spent nuclear fuel
DTN	data tracking number
DS	Drip Shield
EBS	engineered barrier system
EPA	U.S. Environmental Protection Agency
EPRI	Electric Power Research Institute
FAST	Fourier Amplitude Sensitivity Test
FEHM	finite element, heat and mass transfer code
FEIS	Final Environmental Impact Statement
FEP	feature, event, or process
FR	Federal Register

ACRONYMS (Continued)

FTL	FEP Team Lead
HLW	high-level radioactive waste
HTOM	higher-temperature operating mode
IAEA	International Atomic Energy Agency
KTI	Key Technical Issue
LA	License Application
LHS	Latin Hypercube Sampling
LTOM	lower-temperature operating mode
M&O	Management and Operating Contractor
MSTH	multi-scale thermal-hydrologic
NEA	Nuclear Energy Agency
NRC	U.S. Nuclear Regulatory Commission
OECD	Organisation for Economic Co-operation and Development
PA	Performance Assessment
PASS	Performance Assessment Strategy and Scope
PDF	probability distribution function
PMR	process model report
PSHA	probabilistic seismic hazard analysis
PTL	Parameter Team Lead
QA	Quality Assurance
RH	relative humidity
RMEI	reasonably maximally exposed individual
SCC	stress corrosion cracking
SCM	Software Configuration Management
SME	subject matter expert
SR	Site Recommendation
SRC	standardized regression coefficient
SSPA	Supplemental Science and Performance Analysis

ACRONYMS (Concluded)

STN	software tracking number
SZ	saturated zone
TBD	to be determined
TDMS	Technical Data Management System
TER	Technical Error Report
THC	thermal-hydrologic-chemical
TSPA	Total System Performance Assessment
TSPAI	Total System Performance Assessment Integration
UZ	Unsaturated Zone
VA	Viability Assessment
WAPDEG	Waste Package Degradation code
WF	Waste Form
WP	Waste Package
YMP	Yucca Mountain Project

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APPENDIX B

NRC/DOE KTI AGREEMENTS ADDRESSED IN THIS DOCUMENT

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APPENDIX B NRC/DOE KTI AGREEMENTS ADDRESSED IN THIS DOCUMENT

Several TSPAI KTI agreements are addressed in this document, including TSPAI 1.01, 1.02, 4.01, 4.03, and 4.05 (Meserve 2001 [156977]). The agreements and the location of the discussion in this document are provided below.

TSPAI 1.01–DOE will provide enhanced descriptive treatment for presenting barrier capabilities in the final approach for demonstrating multiple barriers. DOE will also provide discussion of the capabilities of individual barriers, in light of existing parameter uncertainty (e.g., in barrier and system characteristics) and model uncertainty. This agreement is addressed in Section 8.3.

TSPAI 1.02–DOE will provide a discussion of the following in documentation of barrier capabilities and the corresponding technical bases: (1) parameter uncertainty, (2) model uncertainty (i.e., the effect of viable alternative conceptual models), (3) spatial and temporal variability in the performance of the barriers, (4) independent and interdependent capabilities of the barriers (e.g., including a differentiation of the capabilities of barriers performing similar functions), and (5) barrier effectiveness with regard to individual radionuclides. DOE will also analyze and document barrier capabilities, in light of existing data and analyses of the performance of the repository system. This agreement is addressed in Section 8.3.

TSPAI 4.01–DOE will document the methodology that will be used to incorporate alternative conceptual models into the performance assessment. The methodology will ensure that the representation of alternative conceptual models in the TSPA does not result in an underestimation of risk. DOE will document the guidance given to process-level experts for the treatment of alternative models. The implementation of the methodology will be sufficient to allow a clear understanding of the potential effect of alternative conceptual models and their associated uncertainties on the performance assessment. This agreement is addressed in Section 3.3.

TSPAI 4.03–DOE will document the method that will be used to demonstrate that the overall results of the TSPA are stable. DOE will provide documentation that submodels (including submodels used to develop input parameters and transfer functions) are also numerically stable. DOE will address in the method the stability of the results with respect to the number of realizations. DOE will describe in the method the statistical measures that will be used to support the argument of stability. The results of the analyses will be provided in the TSPA (or other appropriate documentation) for any potential license application. This agreement is addressed in Section 7.3.

TSPAI 4.05–DOE will document the process used to develop confidence in the TSPA models. The detailed process is currently documented in the model development procedures that are being evaluated for process improvement in response to the model validation corrective action report (CAR-BSC-01-C-001). This agreement is mentioned in Section 7.3.

APPENDIX C

TSPA-LA MODEL DOCUMENT OUTLINE

APPENDIX C TSPA-LA MODEL DOCUMENT OUTLINE

Note: The individual submodel sections (e.g., 6.2.x.y) will have a brief overview similar to that in the TSPA-SR Model AMR, and then text that points the reader to Section 4 for inputs, the appropriate Section 5 subsection for assumptions, and to container(s) in a GoldSim Dashboard file (able to browse using the GoldSim Player software) where the details of the model will be discussed.

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APPENDIX D

TSPA-LA ANALYSIS DOCUMENT OUTLINE

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APPENDIX D TSPA-LA ANALYSIS DOCUMENT OUTLINE

1. PURPOSE
   -Sections 1.1 to 1.3 of TSPA-SR
   -Sections 1.6 to 1.7 of TSPA-SR

2. QUALITY ASSURANCE

3. USE OF SOFTWARE
   -list all software and status

4. INPUTS

4.1 DATA AND PARAMETERS
   -list data/parameters. Significant referencing to Model Document.
4.2 CRITERIA
4.3 CODES AND STANDARDS

5. ASSUMPTIONS

6. SCIENTIFIC ANALYSIS DISCUSSION
   -Section 2 through 2.1.2 of TSPA-SR
6.1 METHOD
   -Section 2.2.4 through 2.2.5.2, and 2.2.5.5 of TSPA-SR
6.2 ANALYSES - NOMINAL SCENARIO CLASS
   -Section 4.1 of TSPA-SR
6.3 ANALYSES – IGNEOUS SCENARIO CLASS
   -Section 4.2 of TSPA-SR
6.4 ANALYSES – SEISMIC SCENARIO CLASS
6.5 ANALYSES – COMBINED SCENARIO CLASSES
   -Section 4.3 of TSPA-SR
6.6 SENSITIVITY ANALYSES
   -uncertainty importance analyses – Section 5.1 from TSPA-SR
6.7 ANALYSES – GROUNDWATER PROTECTION

7. CONCLUSIONS

8. REFERENCES
8.1 DOCUMENTS CITED
8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES
8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

9. ATTACHMENTS

ATTACHMENT A ACRONYMS/GLOSSARY

ATTACHMENT B ALTERNATIVE CONCEPTUAL MODEL DESCRIPTION SUMMARY

Note: Where TSPA-SR sections are identified, the TSPA-LA will have similar sections to the content in that particular section of the TSPA-SR.

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APPENDIX E

TSPA-LA SIMULATION LIST

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APPENDIX E TSPA-LA SIMULATION LIST

E.1 TESTING SIMULATIONS (VALIDATION AND CONFIDENCE BUILDING)

The initial simulations to be performed will be those involving testing. Testing simulations are broken into discretization testing and process testing. Discretization testing (see Table E.1-1) is broken into three major areas: spatial discretization (supports the determination of the number of source term groups), temporal discretization (time step size(s) related to numerical convergence and resolution of peaks), stochastic discretization (number of realizations, and random number seed). These analyses will be documented in the TSPA-LA Model Document.

Table E.1-1. Discretization Test Simulations

Discretization Test Simulations	Nominal	Igneous Groundwater Release	Volcanic Eruptive Release	Seismic
Temporal discretization coarser time steps finer time steps	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr
Spatial discretization fewer source term groups additional source term groups	0 – 10,000 yr	0 – 10,000 yr	n/a*	0 – 10,000 yr
Stochastic discretization Number of realizations 300 realizations 500 realizations 1000 realizations 2000 realizations	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr
Stochastic discretization Random number seed five or more replicates for “x” number of realizations	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr

Note: * The dose rate from the igneous eruptive release modeling case is not a function of the number of waste package groups.

Once the appropriate time step size, number of source term groups, number of realizations, and random number seed have been determined, process testing simulations will be run. These tests will demonstrate the correct performance of the submodels that make up the TSPA model. These analyses will also be documented in the TSPA-LA Model Document.

Table E.1-2. Examples of Process Testing Simulations

Model	Description
Simplified Model	Put all waste packages in a single source term group. Use a simplified WP failure curve. Apply one constant seepage flow rate. Fix chemical parameters (e.g., pH, I, etc.) to constant values.
Full Model	Continuous Release Apply a continuous radionuclide release rate to the WP, invert, UZ, or SZ.
Full Model	Pulse Release Apply a pulse radionuclide release rate to the WP, invert, UZ, or SZ.
Submodel Tests	Exercise a submodel over its range of inputs.
Single Realization	Run a single realization whose behavior is representative of the median, 5^{th}, and/or 95^{th} percentile dose rate curve. Save all simulation results so that the mechanistic behavior of the model can be examined.

The simulations listed in Table E.1-2 would be run for all of the base cases where applicable. Also, the above are only a subset of the process testing that will be done; additional process testing simulations may be developed, and different variations of the tests could be considered.

E.2 BASE CASE SIMULATIONS

Base case simulations will be run for each TSPA scenario class (e.g., nominal, igneous groundwater release, igneous eruptive release, seismic). A base case simulation with a duration of the regulatory time period (10,000 years) will be run for each scenario class, as will a simulation with a duration to 20,000 years to demonstrate that the model results have no major changes after the regulatory time period (see Table E.2-1). These analyses will be documented in the TSPA-LA Analysis Document, and the 10,000 year results are expected to be documented in the License Application itself.

Table E.2-1. Base Case Simulations

Scenario Class	Duration
Nominal	0 – 10,000 years 0 – 20,000 years
Igneous Groundwater Release	0 – 10,000 years 0 – 20,000 years
Volcanic Eruptive Release	0 – 10,000 years 0 – 20,000 years
Seismic	0 – 10,000 years 0 – 20,000 years

E.3 SEQUENTIAL ONE-ON BARRIER/PROCESS SIMULATIONS

Table E.3-1 contains an example of one set of sequential one-on barrier/process simulations for the nominal scenario class. Additional simulations may be run for igneous/groundwater release modeling case and the seismic scenario class. Also, the barriers/processes could be added in a variety of different orders, different treatments of the barriers/processes could be considered, and additional processes/barriers could be considered. These analyses will be documented in the TSPA-LA Model Document.

Table E.3-1. Example of a Nominal Case Set of Sequential One-On Barrier/Process Simulations

Process Addition	Description
3,000 acre-feet	The assumption is that radionuclides cannot reach humans or biosphere without first being buffered by the 3000 acre-feet volume. For this case, assume infinite solubilities with entire inventory dissolved in 3000 acre-feet volume. Waste is assumed to be in powder form.
partial waste-form	Waste is now assumed to be in rod and glass-log form and sitting bare on the surface of the mountain (or at the repository level, but with the top of the mountain removed). But now the waste dissolves slowly according to the CSNF and codisposal degradation rates, but with infinite solubility and maximum colloids.
full waste-form	Add solubility/concentration limits for dissolved, irreversible, and reversible radionuclides.
precipitation/climate	Limited transport rate to the 3000 acre-feet biosphere (i.e., limited by the rate of advection at the precipitation rate).
infiltration/surficial soil barrier/decay heat	Soil layer and evapo-transpiration limit water ingress to the mountain.
seepage	Further limitation of flux of water contacting waste due to presence of drifts and fracture-matrix heterogeneity in the TSw.
UZ barrier	Add unsaturated zone flow and transport.
SZ barrier	Add saturated zone flow and transport.
cladding barrier	Add cladding as a barrier.
drip shield barrier	Add drip shields.
invert barrier	Add invert, including its corrosion products.
waste package barrier	Add waste packages.

E.4 BARRIER/PROCESS NEUTRALIZATION

Table E.4-1 contains examples of barrier/process neutralization simulations. They would be performed for both the nominal and igneous groundwater release base cases by modifying the TSPA model. Barrier/process neutralization simulations may be developed for the volcanic eruptive release modeling case and seismic scenario class. Also, different ways of "neutralizing" the barriers/processes could be considered, and additional processes/barriers could be considered. Combinations of barriers may also be neutralized (e.g., two or more at a time rather than just one at a time). These analyses will be documented in the TSPA-LA Model Document.

Table E.4-1. Examples of Barrier/Process Neutralization Simulations

Barrier	Barrier/Process to be Modified
Waste Package	Neutralize the waste package
Drip Shield	Neutralize the drip shield
Engineered Barrier System	Neutralize the invert
Unsaturated Zone	Neutralize seepage
Waste Form	Neutralize solubility
Engineered Barrier System/Waste Package	Neutralize EBS and WP K_ds
Unsaturated Zone	Neutralize the UZ
Saturated Zone	Neutralize the SZ

E.5 DSNF AND NAVAL FUEL SENSITIVITY SIMULATIONS

Table E.5-1 contains examples of DSNF and Naval fuel sensitivity simulations. They would be performed for both the nominal and igneous groundwater release base cases. Simulations may also be developed for the igneous eruptive release modeling case and seismic scenario class. The current categorization of DSNF would result in 10 additional sensitivity analyses using the TSPA model. These analyses will be documented in the TSPA-LA Analysis Document.

Table E.5-1. Examples of DSNF and Naval Fuel Sensitivity Simulations

Fuel Type	Base Case Inventory Replacement
Naval	fuel source term release rate[1]
DSNF	inventory type 2 – Pu/U alloy
DSNF	inventory type 3 – Pu/U carbide
DSNF	inventory type 4 – MOX/Pu oxide
DSNF	inventory type 5 – Th/U carbide
DSNF	inventory type 6 – Th/U oxide
DSNF	inventory type 7 – Uranium metal
DSNF	inventory type 8 – Uranium oxide
DSNF	inventory type 9 – Al-based SNF
DSNF	inventory type 10 – U Nitride SNF
DSNF	inventory type 11 – U-Zirconium hydride

1 The naval fuel source term will be supplied by Naval Reactors and documented in a classified report. An unclassified summary will be provided to the DOE.

APPENDIX F

EXAMPLE TSPA-LA INPUT PARAMETER TABLE

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APPENDIX F EXAMPLE TSPA-LA INPUT PARAMETER TABLE

Tables of input parameters for the TSPA-LA model will be produced as part of the TSPA-LA Model Document. Table F-1 provides an example which illustrates the information that will be captured in these tables. Note that the information in this table is illustrative and may not reflect the final input parameters and/or sources used in the TSPA-LA model.

Table F-1. Seepage Input Parameters to the TSPA-LA Model (example)

Input Parameter	Description	Location	Abstraction Source	DTN Source	Uncertain/ Constant
Episodic_Factor	episodic factor	\TSPA_Model\Engineered_Barrier_System\Drift_Seepage\Seepage_DLL_Inputs\	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
Flow_Focus_Factor_Distribution	flow focus factor	\TSPA_Model\Engineered_Barrier_System\Drift_Seepage\Seepage_DLL_Inputs\	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
mean seepage flow rate	mean seepage flow rate distribution as a function of percolation flux	input file: SeepFlowMean.dat	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
Seep_Uncertainty	seepage uncertainty for seepage fraction, mean seepage flow rate, and seepage flow rate std. dev.	\TSPA_Model\Engineered_Barrier_System\Drift_Seepage\Seepage_DLL_Inputs\	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
seepage flow rate std.dev.	seepage flow rate standard deviation distribution as a function of percolation flux	input file: SeepFlowSD.dat	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
seepage fraction	seepage fraction distribution as a fuction of percolation flux	input file: SeepFrac.dat	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
percolation flux	Percolation flux time-history 5 m from the crown of the drift. A set of percolation flux time-histories is provided for each infiltration scenario (low, mean, high) and for each infiltration bin that exist in a given infiltration scenario.	input files: CSNF_HT_high_pf_bin2.txt CSNF_HT_high_pf_bin3.txt CSNF_HT_high_pf_bin4.txt CSNF_HT_high_pf_bin5.txt CSNF_HT_low_pf_bin1.txt CSNF_HT_low_pf_bin2.txt CSNF_HT_mean_pf_bin2.txt CSNF_HT_mean_pf_bin3.txt CSNF_HT_mean_pf_bin4.txt CSNF_LT2_high_pf_bin2.txt CSNF_LT2_high_pf_bin3.txt CSNF_LT2_high_pf_bin4.txt CSNF_LT2_high_pf_bin5.txt CSNF_LT2_low_pf_bin1.txt CSNF_LT2_low_pf_bin2.txt CSNF_LT2_mean_pf_bin2.txt CSNF_LT2_mean_pf_bin3.txt CSNF_LT2_mean_pf_bin4.txt HLW_HT_high_pf_bin2.txt HLW_HT_high_pf_bin3.txt	ANL-EBS-MD-00049, REV01 DRAFT	TBD	constant

Table F-1. Seepage Input Parameters to the TSPA-LA Model (example) (Continued)

Input Parameter	Description	Location	Abstraction Source	DTN Source	Uncertain/ Constant
percolation flux	Percolation flux time-history 5 m from the crown of the drift. A set of percolation flux time-histories is provided for each infiltration scenario (low, mean, high) and for each infiltration bin that exist in a given infiltration scenario.	HLW_HT_high_pf_bin4.txt HLW_HT_high_pf_bin5.txt HLW_HT_low_pf_bin1.txt HLW_HT_low_pf_bin2.txt HLW_HT_mean_pf_bin2.txt HLW_HT_mean_pf_bin3.txt HLW_HT_mean_pf_bin4.txt HLW_LT2_high_pf_bin2.txt HLW_LT2_high_pf_bin3.txt HLW_LT2_high_pf_bin4.txt HLW_LT2_high_pf_bin5.txt HLW_LT2_low_pf_bin1.txt HLW_LT2_low_pf_bin2.txt HLW_LT2_mean_pf_bin2.txt HLW_LT2_mean_pf_bin3.txt HLW_LT2_mean_pf_bin4.txt	ANL-EBS-MD-00049, REV01 DRAFT	TBD	constant

APPENDIX G

TSPA-LA DOCUMENT HIERARCHY

APPENDIX G TSPA-LA DOCUMENT HIERARCHY

The TSPA-LA will rely on numerous supporting documents for information and abstractions. A representation of the primary supporting documents for the following components is presented in the figures of this appendix (Figures G-1 through G-10): 1) UZ flow, 2) EBS environment, 3) waste package and drip shield degradation, 4) waste form degradation and mobilization, 5) EBS flow and transport, 6) UZ transport, 7) SZ flow and transport, 8) biosphere, 9) disruptive events igneous scenario class, and 10) disruptive events seismic scenario class. The document hierarchy is evolving, so these diagrams are intended to be illustrative and provide a general view of the main documents supporting TSPA-LA. Since the documentation is only proposed and is currently under development, the document identifiers are listed where available, but no DIRS are linked to this appendix. The Legend for the figures is shown below. Table G-1 presents a listing of some of the key documents that are expected to support TSPA-LA.

Note that the diagrams presented in this appendix reflect how information flows among the documentation that supports the development of each TSPA model component. The information flow presented in this context is generally not the same as the information flow between models in the TSPA model as depicted in Figure 5.1-1. In the former case, the information flow supports model development and analyses, whereas in the latter case, information flow enables model implementation. Also, note that the design and data feeds are not included on these diagrams. Finally, note that the "supporting AMR" boxes indicate documents that don't directly provide inputs to the TSPA model for that particular component. They may directly feed TSPA in another component.

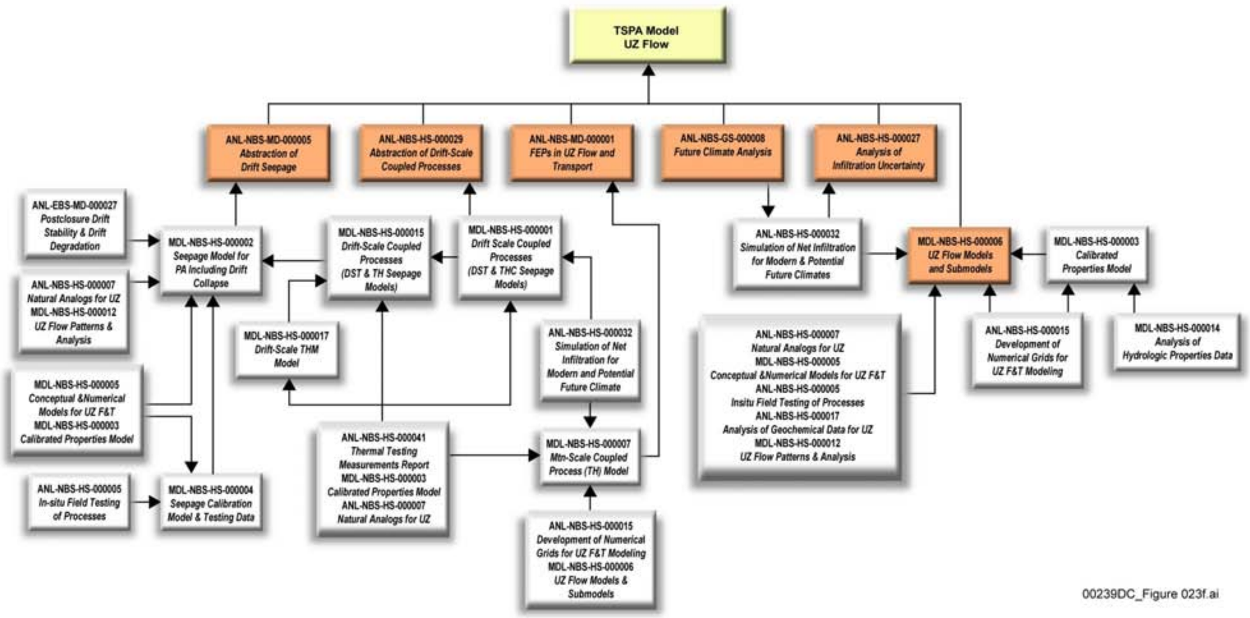

Figure G-1. Unsaturated Zone Flow Document Hierarchy

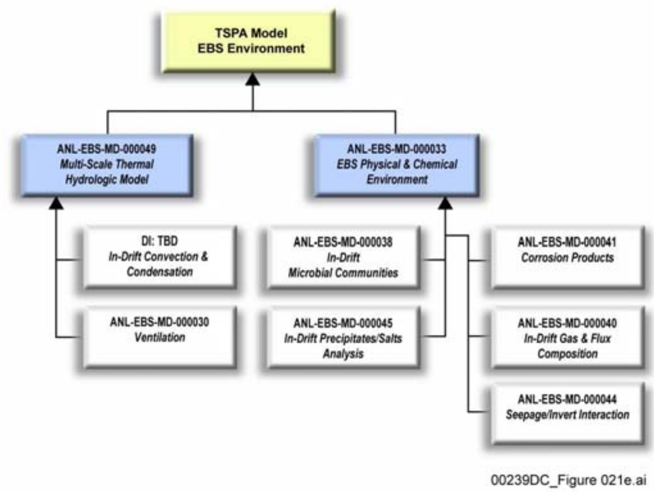

Figure G-2. EBS Environment Document Hierarchy

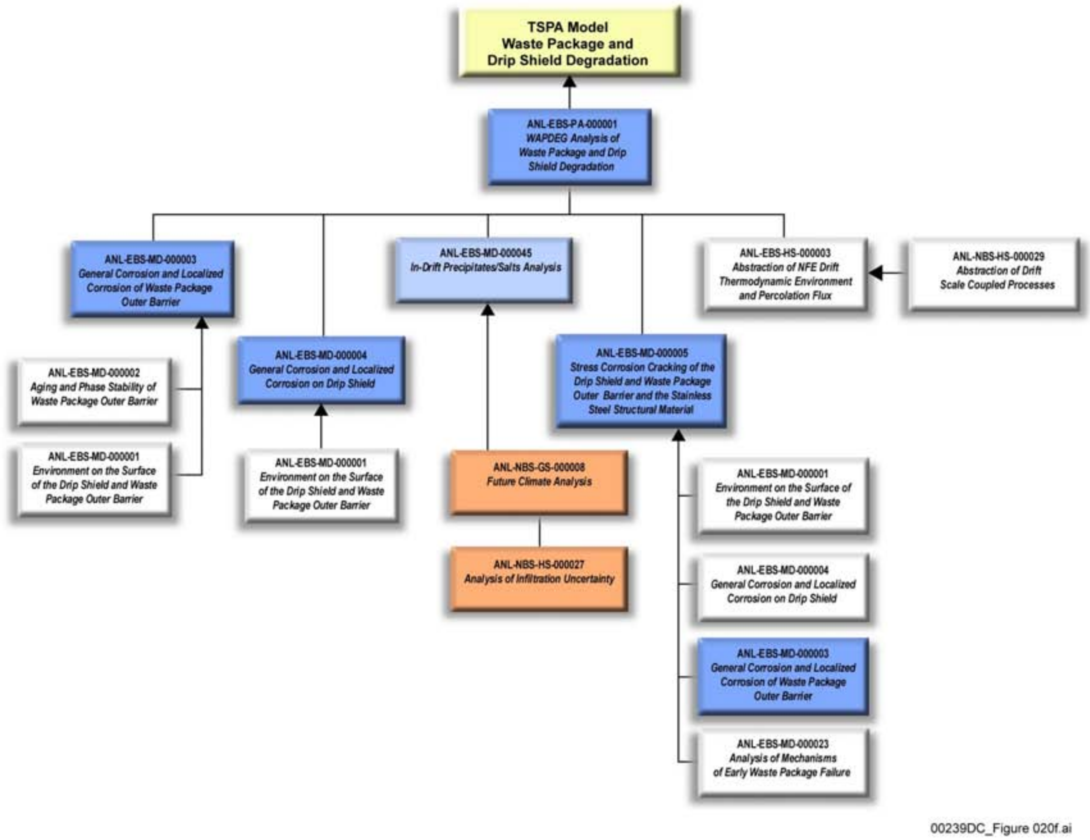

Figure G-3. Waste Package and Drip Shield Degradation Document Hierarchy

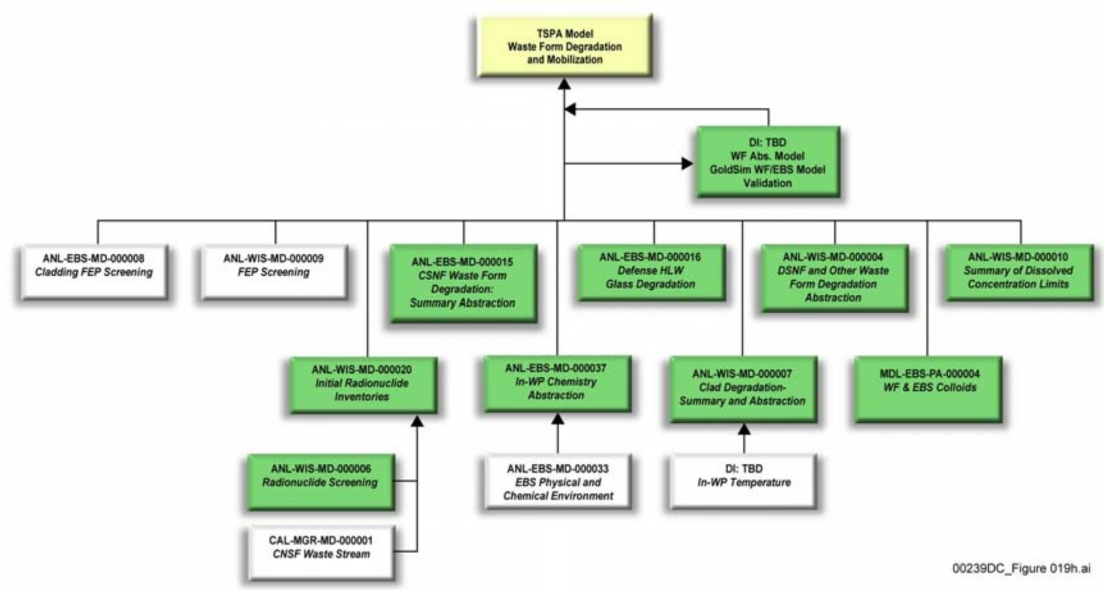

Figure G-4. Waste Form Degradation and Mobilization Document Hierarchy

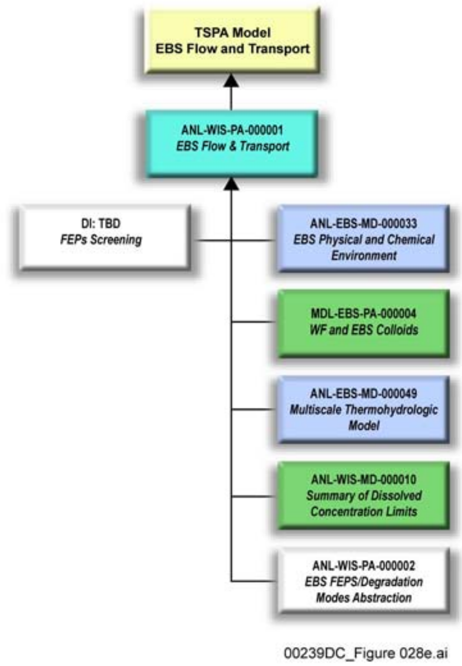

Figure G-5. Engineered Barrier System Flow and Transport Document Hierarchy

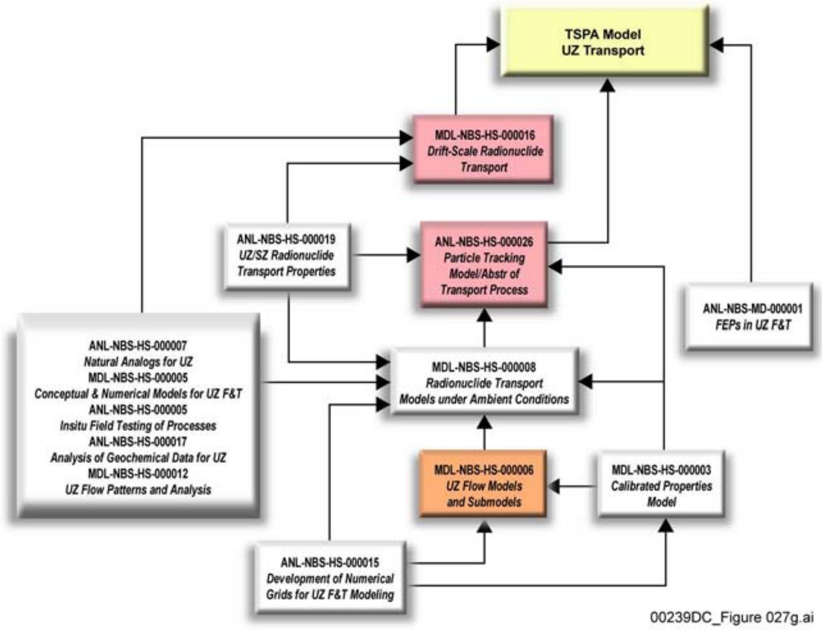

Figure G-6. Unsaturated Zone Transport Document Hierarchy

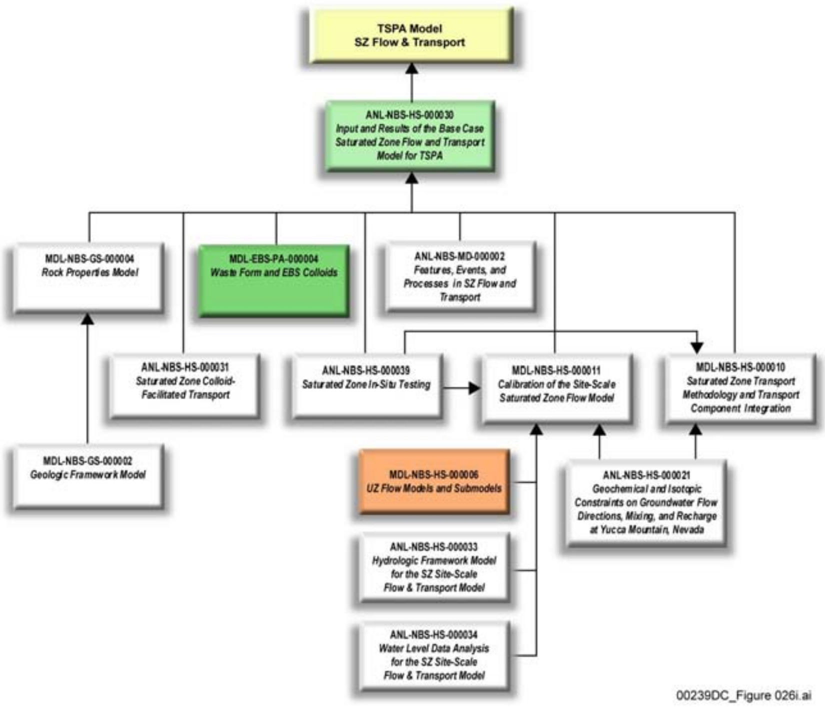

Figure G-7. Saturated Zone Flow and Transport Document Hierarchy

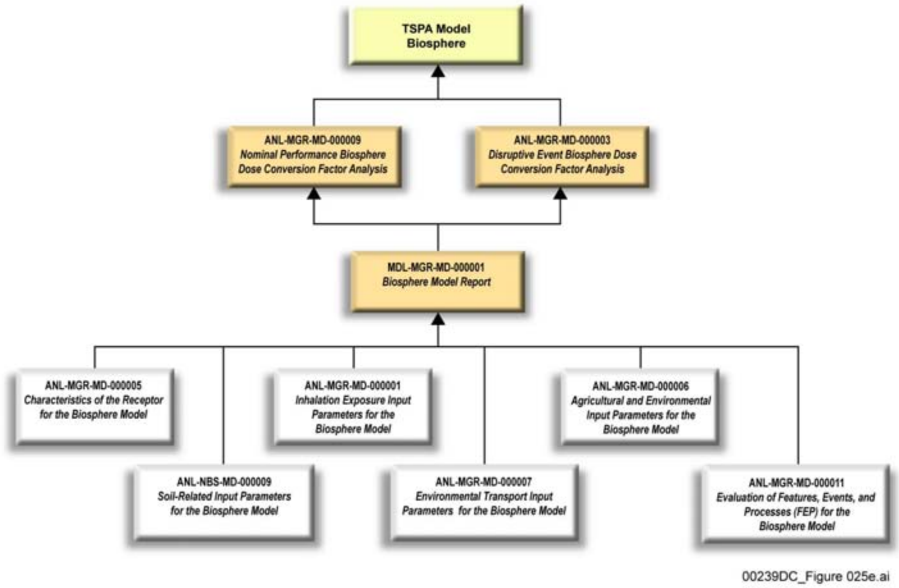

Figure G-8. Biosphere Document Hierarchy

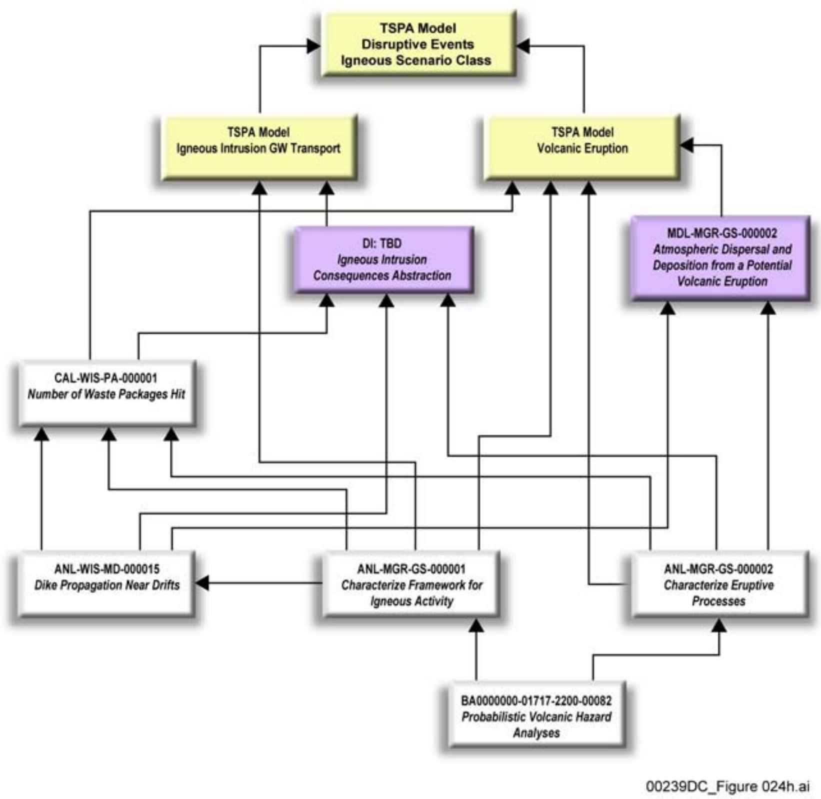

Figure G-9. Disruptive Events Igneous Scenario Class Document Hierarchy

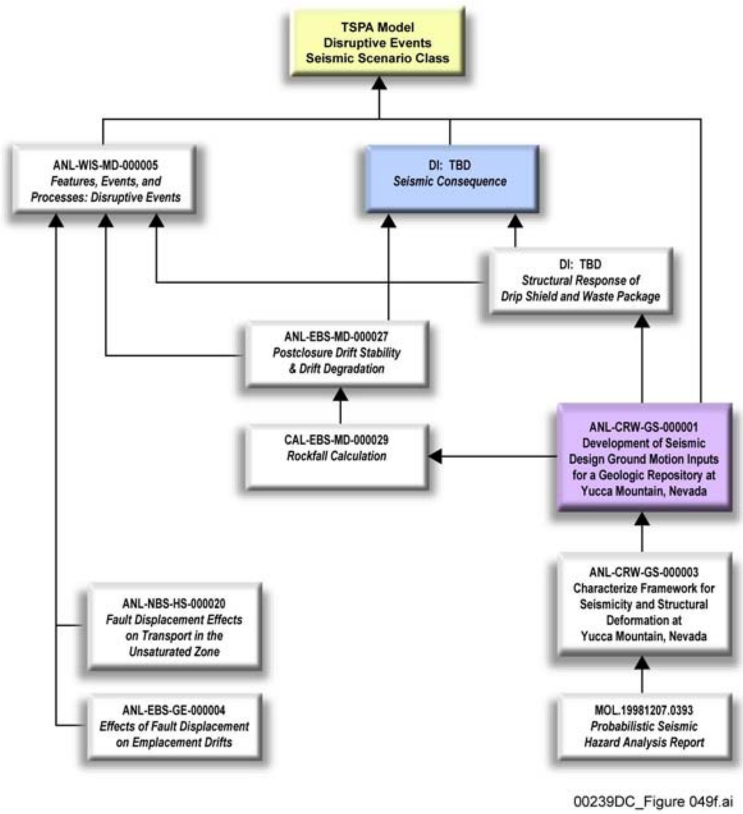

Figure G-10. Disruptive Events Seismic Scenario Class Document Hierarchy

Table G-1. Key Documents that Directly Support TSPA-LA

Model	Document Title	Doc. ID	Document Control ID
Unsaturated Zone Flow			
Climate	Future Climate Analysis	U0005	ANL-NBS-GS-000008
Infiltration	Analysis of Infiltration Uncertainty	U0095	ANL-NBS-HS-000027
Mountain-Scale Flow Model	UZ Flow Models and Submodels	U0050	MDL-NBS-HS-000006
Drift Seepage	Abstraction of Drift Seepage	U0120	ANL-NBS-MD-000005
Drift Scale Coupled Processes	Abstraction of Drift Scale Coupled Processes	N0125	ANL-NBS-HS-000029
EBS Environment			
EBS Thermal-Hydrologic Environment	Multiscale Thermohydrologic Model	E0120	ANL-EBS-MD-000049
EBS Chemical Environment	EBS Physical & Chemical Environment Model	E0100	ANL-EBS-MD-000033
	In-Drift Precipitates/Salts Analysis	E0105	ANL-EBS-MD-000045
Waste Package and Drip Shield Degradation			
Waste Package and Drip Shield Degradation	WAPDEG Analysis of Waste Package and Drip Shield Degradation	W0050	ANL-EBS-PA-000001
Waste Package General and Localized Corrosion	General Corrosion and Localized Corrosion of Waste Package Outer Barrier	W0035	ANL-EBS-MD-000003
Drip Shield General and Localized Corrosion	Generalized Corrosion and Localized Corrosion on Drip Shield	W0085	ANL-EBS-MD-000004
Stress Corrosion Cracking of Waste Package and Drip Shield	SCC of Drip Shield and Waste Package Outer Barrier and the Stainless Steel Structural Material	W0095	ANL-EBS-MD-000005
Waste Form Degradation and Mobilization			
Radionuclide Inventory	Radionuclide Screening	F0015	ANL-WIS-MD-000006
	Initial Radionuclide Inventories	F0016	ANL-WIS-MD-000020
In-Package Chemistry	In- Package Chemistry Abstraction	F0170	ANL-EBS-MD-000037
Cladding Degradation	Clad Degradation - Summary and Abstraction	F0155	ANL-WIS-MD-000007
Waste Form Degradation	CSNF Waste Form Degradation: Summary Abstraction	F0055	ANL-EBS-MD-000015
	Defense HLW Glass Degradation	F0060	ANL-EBS-MD-000016
	DSNF and Other Waste Form Degradation Abstraction	F0065	ANL-WIS-MD-000004
Dissolved Radionuclide Concentration Limits	Summary of Dissolved Concentration Limits	F0095	ANL-WIS-MD-000010
Waste Form and EBS Colloids	Waste Form and EBS Colloids	F0115	MDL-EBS-PA-000004
EBS Flow and Transport			
EBS Flow and Transport	EBS Flow and Transport	E0095	ANL-WIS-PA-000001
Unsaturated Zone Transport			
UZ Particle Tracking	Particle Tracking Model/Abstraction of Transport Process	U0065	ANL-NBS-HS-000026
Drift Scale Radionuclide Transport	Drift-Scale Radionuclide Transport	U0230	MDL-NBS-HS-000016
Saturated Zone Flow and Transport			
SZ Convolution	SZ Transport Abstractions	S0055	ANL-NBS-HS-000030
1D SZ Transport	SZ Transport Abstractions	S0055	ANL-NBS-HS-000030
SZ Flow and Transport	SZ Transport Abstractions	S0055	ANL-NBS-HS-000030

Table G-1. Key Documents that Directly Support TSPA-LA (Continued)

Model	Document Title	Doc. ID	Document Control ID
Biosphere			
Biosphere	Biosphere Model Report	B0090	MDL-MGR-MD-000001
	Nominal Performance Biosphere Dose Conversion Factor Analysis	B0065	ANL-MGR-MD-000009
	Disruptive Event Biosphere Dose Conversion Factor Analysis	B0055	ANL-MGR-MD-000003
Disruptive Events			
Seismic Activity	Seismic Consequence	TBD	TBD
Igneous Intrusion	Igneous Intrusion Consequences Abstraction	TBD	TBD
Volcanic Eruption	Atmospheric Dispersal and Deposition from a Potential Volcanic Eruption	T0125	MDL-MGR-GS-000002